

=> S 11 and L3
 40511 L1
 13647 L3
 L4
 31 L1 AND L3

=> S 14 and (racemi? or resol?)

39218 RACEMI?
 442012 RESOL?

L5
 23 L4 AND (RACEMI? OR RESOL?)

=> d 1-23 ibib abs hitstr

L5 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2004 ACS ON STN
 ACCESSION NUMBER: 2003:417577 CAPLUS
 DOCUMENT NUMBER: 139:6672

TITLE: Process for the synthesis of (R)-1-(3,5-bis(trifluoromethyl)phenyl)ethan-1-ol and esters thereof by dynamic kinetic resolution

INVENTOR(S): Karel Maria Broxterman, Quirinus Bernardus; Verzijl, Gerardus Merck & Co., Inc., USA

PATENT ASSIGNEE(S): PCT Int. Appl., 44 pp.

SOURCE: CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM: COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003043575	A2	20030530	WO 2002-US36969	20021115
WO 2003043575	A3	20031016		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MN, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-333039P P 20011119

OTHER SOURCE(S): CASREACT 139:6672; MARPAT 139:6672

AB (R)-1-(3,5-bis(trifluoromethyl)phenyl)ethan-1-ol and esters thereof were obtained via dynamic kinetic resoln. These compds. are useful as intermediates in the synthesis of compds. which possess pharmacol. activity. Thus, 1,3-(F3C)2C6H4 was brominated and the resulting 3,5-(F3C)3C6H3Br subjected to Grignard reaction with Ac2O to give 3,5-(F3C)3C6H3COMe or with MeCHO to give 3,5-(F3C)3C6H3CHMeOH. 3,5-(F3C)3C6H3COMe was subjected to transfer hydrogenation in presence of [RuCl2(p-cymene)]2 and (R,S)-H2NCMePhCONH2 to give (R,S)-3,5-(F3C)3C6H3CHMeOH which was subjected to kinetic resoln. with CH2CMeOAc in presence of Novozym435 to give (R)-3,5-(F3C)3C6H3CHMeOAc with 99% ee.

IT 9001-62-1, Novozym435 12321-08-3 37362-03-1

37366-09-9, Benzene-ruthenium dichloride dimer 37375-79-4

52462-29-0, p-Cymeneruthenium dichloride dimer 52462-30-3

52462-31-4 67421-02-7 88946-78-5

88946-79-6 88946-80-9 104439-77-2

123265-36-1

RL: CAT (Catalyst use): USES (Uses)

(process for the synthesis of (R)-1-(3,5-bis(trifluoromethyl)phenyl)eth

=> S 11 and L3
 40511 L1
 13647 L3
 L4
 31 L1 AND L3

=> S 14 and (racemi? or resol?)

39218 RACEMI?

442012 RESOL?

L5
 23 L4 AND (RACEMI? OR RESOL?)

=> d 1-23 ibib abs hitstr

L5 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2004 ACS ON STN
 ACCESSION NUMBER: 2003:417577 CAPLUS
 DOCUMENT NUMBER: 139:6672

TITLE: Process for the synthesis of (R)-1-(3,5-bis(trifluoromethyl)phenyl)ethan-1-ol and esters thereof by dynamic kinetic resolution

INVENTOR(S): Karel Maria Broxterman, Quirinus Bernardus; Verzijl, Gerardus Merck & Co., Inc., USA

PATENT ASSIGNEE(S): PCT Int. Appl., 44 pp.

SOURCE: CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM: COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003043575	A2	20030530	WO 2002-US36969	20021115
WO 2003043575	A3	20031016		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MN, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-333039P P 20011119

OTHER SOURCE(S): CASREACT 139:6672; MARPAT 139:6672

AB (R)-1-(3,5-bis(trifluoromethyl)phenyl)ethan-1-ol and esters thereof were obtained via dynamic kinetic resoln. These compds. are useful as intermediates in the synthesis of compds. which possess pharmacol. activity. Thus, 1,3-(F3C)2C6H4 was brominated and the resulting 3,5-(F3C)3C6H3Br subjected to Grignard reaction with Ac2O to give 3,5-(F3C)3C6H3COMe or with MeCHO to give 3,5-(F3C)3C6H3CHMeOH. 3,5-(F3C)3C6H3COMe was subjected to transfer hydrogenation in presence of [RuCl2(p-cymene)]2 and (R,S)-H2NCMePhCONH2 to give (R,S)-3,5-(F3C)3C6H3CHMeOH which was subjected to kinetic resoln. with CH2CMeOAc in presence of Novozym435 to give (R)-3,5-(F3C)3C6H3CHMeOAc with 99% ee.

IT 9001-62-1, Novozym435 12321-08-3 37362-03-1

37366-09-9, Benzene-ruthenium dichloride dimer 37375-79-4

52462-29-0, p-Cymeneruthenium dichloride dimer 52462-30-3

52462-31-4 67421-02-7 88946-78-5

88946-79-6 88946-80-9 104439-77-2

123265-36-1

RL: CAT (Catalyst use): USES (Uses)

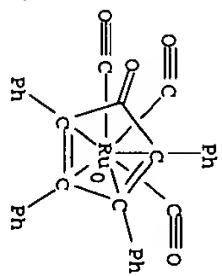
(process for the synthesis of (R)-1-(3,5-bis(trifluoromethyl)phenyl)eth

an-1-ol and esters thereof by dynamic kinetic resoln.)

RN 9001-62-1 CAPLUS
 CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

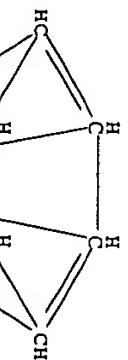
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RN 12321-08-3 CAPLUS
 CN Ruthenium, tricarbonyl[(2,3,4,5--eta.)-2,3,4,5-tetraphenyl]-2,4-cyclopentadien-1-one] (9CI) (CA INDEX NAME)

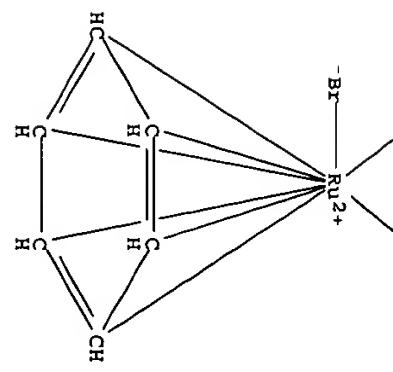


RN 37362-03-1 CAPLUS
 CN Ruthenium, bis(.eta.6-benzene)di-.mu.-bromodibromodi-. (9CI) (CA INDEX NAME)

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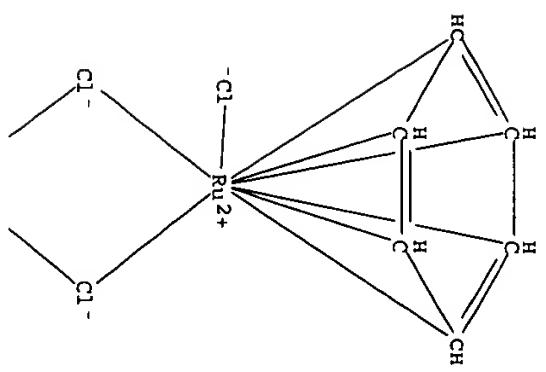


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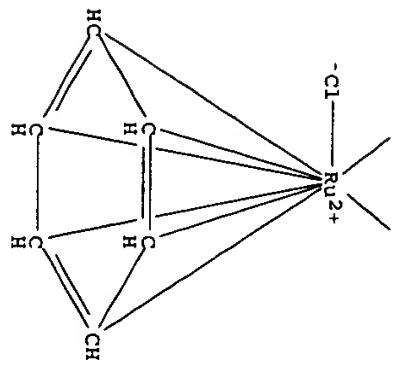


RN 37366-09-9 CAPLUS
CN Ruthenium, bis(.eta.6-benzene)di-.mu.-chlorodichlorodi- (9CI) (CA INDEX
NAME)

PAGE 1-A

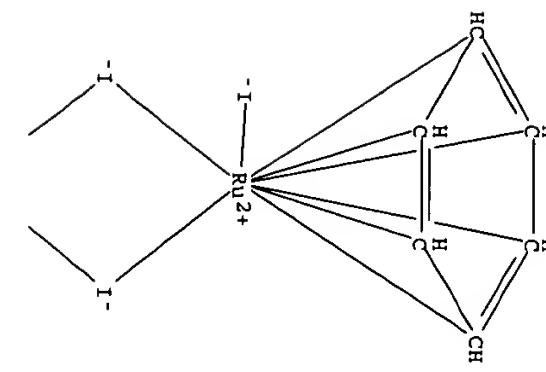


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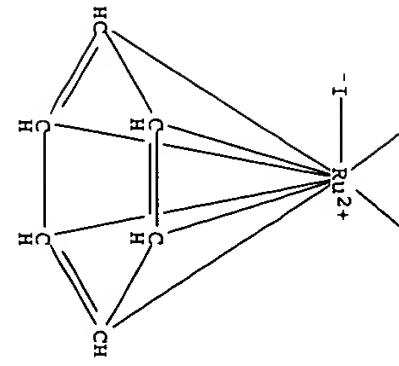


RN 37375-79-4 CAPLUS
CN Ruthenium, bis(.eta.6-benzene)di-.mu.-iododiodo- (9CI) (CA INDEX NAME)

PAGE 1-A

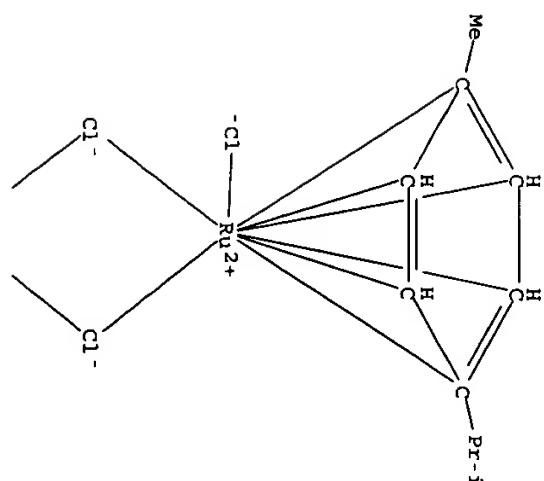


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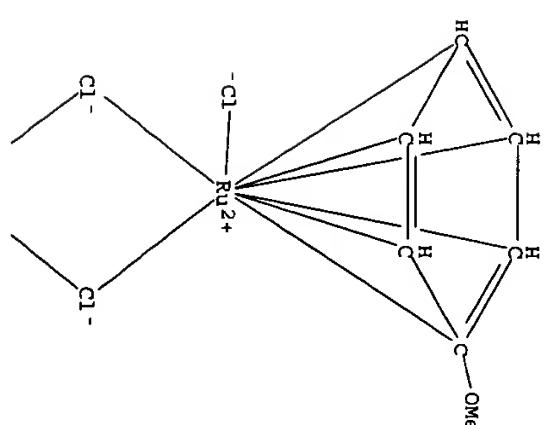
RN 52462-29-0 CAPLUS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)

PAGE 1-A



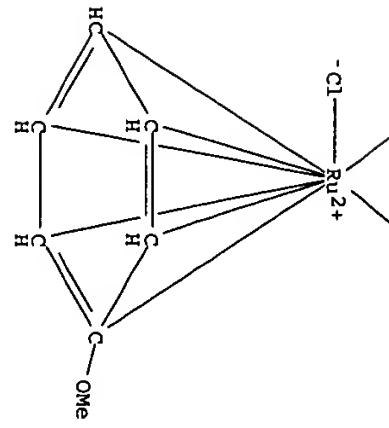
RN 52462-30-3 CAPLUS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-methoxybenzene]di- (9CI) (CA INDEX NAME)

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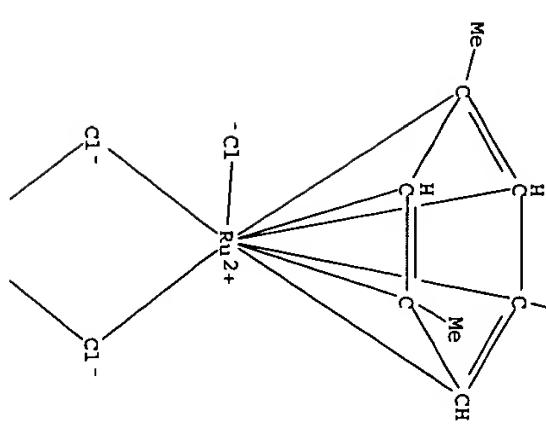
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RN 52462-31-4 CAPLUS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1,3,5-trimethylbenzene]di- (9CI) (CA INDEX NAME)

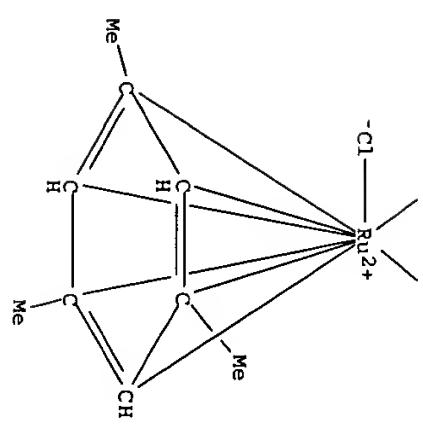
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PAGE 2-A



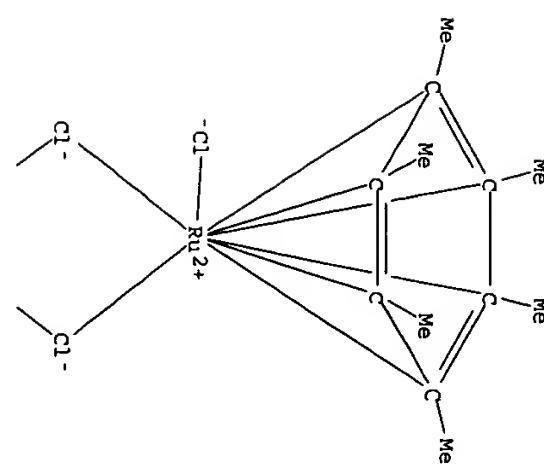
RN 67421-02-7 CAPLUS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-hexamethylbenzene]di- (9CI) (CA INDEX NAME)

Me

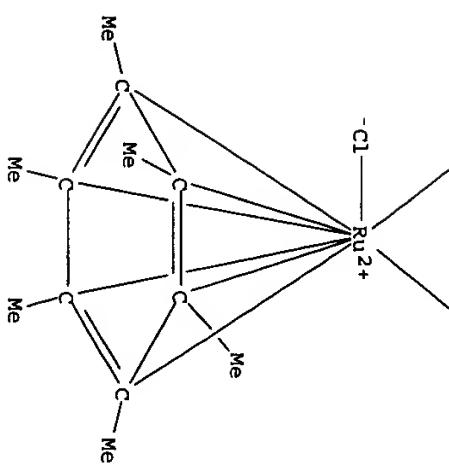


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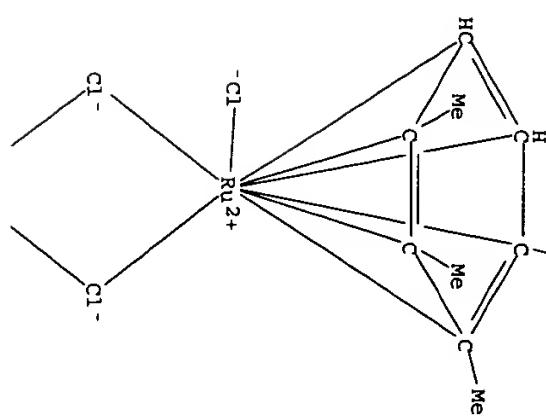
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PAGE 1-A

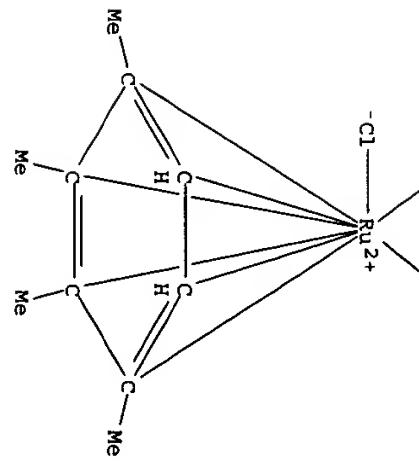


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RN 88946-78-5 CAPLUS
CN Ruthenium, di-*mu*-chlorodichlorobis[(1,2,3,4,5,6-*eta*)-1,2,3,4-tetramethylbenzene]di- (GCI) (CA INDEX NAME)

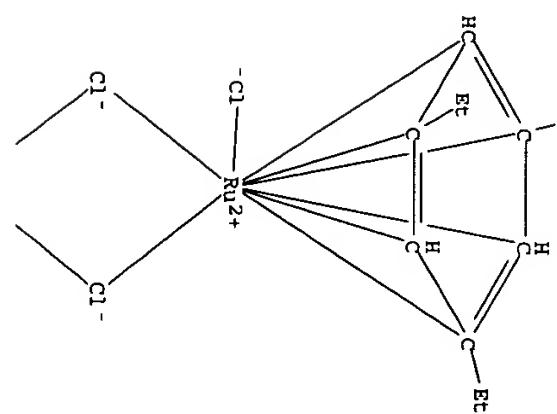
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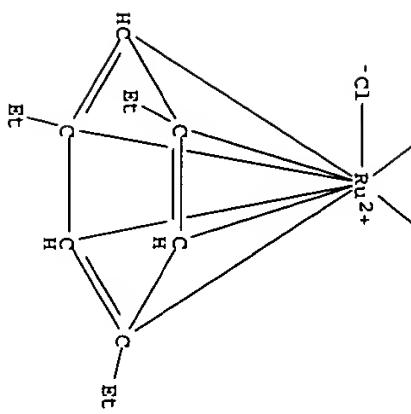
RN 88946-79-6 CAPIUS
CN Ruthenium, di-mu-chlorodichlorobis[(1,2,3,4,5,6-*eta.*)-1,3,5-triethylbenzene di- (9CI) (CA INDEX NAME)

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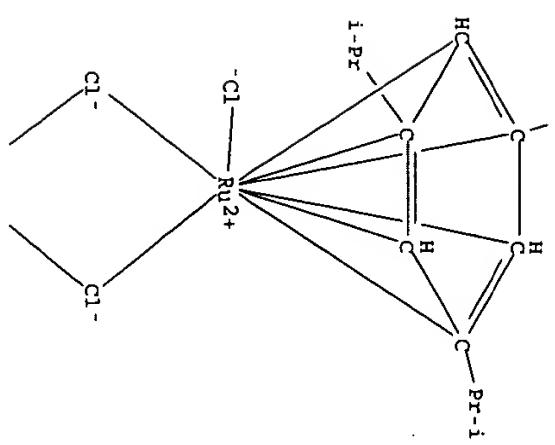


PAGE 3-A



RN 88946-80-9 CAPLUS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1,3,5-tris(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)

PAGE 1-A



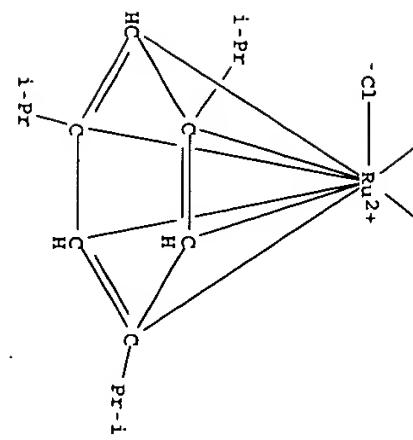
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-Cl

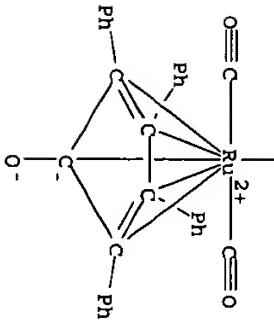
PAGE 2-A

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[({1,2,3,4,5-.eta.})-1-hydroxylato-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]({1,2,3,4,5-.eta.})-1-hydroxy-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl] di- (9CI) (CA INDEX NAME)

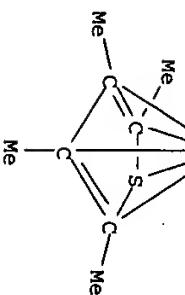
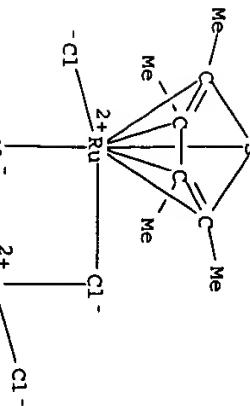
PAGE 3-A



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RN 123265-36-1 CAPTUS
CN Ruthenium, di--mu-chlorodichlorobis[(2,3,4,5-eta.)-tetramethylthiophene--kappa.S]d₂ stereoisomer (9CT) (CA INDEX NAME)



15 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2004 ACS on STW
 ACCESSION NUMBER: 2003:273130 CAPLUS
 DOCUMENT NUMBER: 139:214151
 TITLE: Asymmetric hydrogenation of a
 unsaturated ketone by diamine
 phosphine)ruthenium(II) complex
 kinetic resolution: a consecutive
 Lindner, Ekkehard; Ghani, AB
 Eichele, Klaus; Mayer, Hermann
 Institute of Inorganic Chemistry
 Tubingen, Tubingen, 72075, GE
 Tetrahedron: Asymmetry (2003)
 CODEN: TASYE3; ISSN: 0957-4116
 Elsevier Science Ltd.
 Journal
 DOCUMENT TYPE:
 LANGUAGE: English
 AB The RuCl₂(.eta.1-Ph₂CH₂CH₂CH₃)₂(diamine) complex
 high yields from the reaction of equimolar amounts
 Ph₂CH₂CH₂CH₂CH₃)₂ with various kinds of chelating
 five-membered chelates with ruthenium. These novel

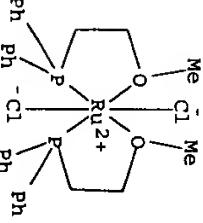
complexes have been used as catalysts in the asym. hydrogentation of the prochiral ketone trans-4-phenyl-3-buten-2-one (1), using 2-propanol and different types of cocatalysts. Whereas complexes with achiral diamines afforded the **racemic** alcs., complexes with chiral diamines (R,R or S,S) allowed the formation of the corresponding enantiomerically enriched secondary alc. (S or R) with ee values of 45%. In order to obtain the secondary alc. with ee of >95%, the kinetic **resoln.** of enantiomerically enriched I was performed in a consecutive approach using either the lipase-catalyzed enantioselective transesterification of the alc. with isopropenyl acetate as the acyl donor in toluene or the enantioselective hydrolysis of the corresponding acetate in buffer. The detn. of the enantiomeric excess (ee) of the resulting enantiomerically enriched secondary alcs. was performed by gas chromatog. using heptakis(2,3-di-O-methyl-6-O-tert-butyldimethylsilyl)-.beta.-cyclodextrin as the chiral stationary phase.

RL: CAT (Catalyst use); USES (Uses)
(asym. hydrogenation of an .alpha., .beta.-unsatd. ketone by
diamine(ether-phosphine)ruthenium(II) complexes and lipase-catalyzed
kinetic resoln.)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Ru: (acu) (reactant); (racu) (reactant or reagent)
 (asym. hydrocarbon) of an α ,-alpha.-unsatd. ketone by
 diamine (ether phosphine) ruthenium(II) complexes and lipase-catalyzed

RN 109011-62-3 CAPLUS
CN Ruthenium, dichlorobis([2-(methoxy-.kappa.0) ethyl]diphenylphosphine-
kinetic reson.)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS

L5 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2003:120380 CAPLUS
DOCUMENT NUMBER: 138:283203

TITLE: On the Mechanism of the Unexpected Facile Formation of meso-Diacetate Products in Enzymatic Acetylation of

Author(s): Alkanediols
Title: Reactions of
Author(s): Michael J. T. R

CORPORATE SOURCE: DOW, MICHIGAN; BAETKAIL, JAHN.

SOURCE: Stockholm University, Stockholm, SE-106 91, Sweden.
Journal of Organic Chemistry (2003), 68(6), 2216-2222

PUBLISHER: American Chemical Society
CODEN: JOCEAH; ISSN: 0822-3263

DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:283203
AB The mechanism of the unexpected facile formation of meso-diacetate

previously obsd. in the enzymic resoln. of DL/meso mixts. of

high yields from the reaction of equimolar amounts of $\text{RuCl}_2 \cdot \text{eta} \cdot 2\text{-Ph}_2\text{PCH}_2\text{CH}_2\text{OEt}_3$ with various kinds of chelating diamines to form five-membered chelates with ruthenium. These novel ruthenium(III)

2,4-pentanediol and 2,5-hexanediol with *Candida antarctica* lipase B has been elucidated. It was found that the formation of meso-diacetate proceeds via different mechanisms for the two diols. Enzyme-catalyzed acylation of Aco-d3 labelled (R)-monoacetates of meso-2,4-pentanediol and meso-2,5-hexanediol and anal. of the meso-diacetates obtained show that the former reaction proceeds via intramol. acyl migration while the latter occurs via direct S-acylation of the alc. For the (R)-monoacetate of (R,S)-2,4-pentanediol the intramol. acyl migration was fast and therefore direct S-acylation by the external acyl donor is suppressed. For the hexanediol monoacetate the rate ratio (pseudo E value) between (5R,2R)- and (5R,2S)-5-acetoxy-2-hexanol was exptl. detd. to be KR, R/KR, S = 25, which is about 10-20 times lower than the E value for 2-pentanol and 2-octanol. In a preliminary expt. it was demonstrated that facile acyl migration in the 1,3-diol deriv. can be utilized to prep.

syn-1,3-diacetoxyxynane (>90% syn) in high enantioselectivity (>99% ee)

via a chemoenzymic dynamic kinetic asym. transformation of a meso/DL mixt. of 1,3-nanediol.

IT 104439-77-2

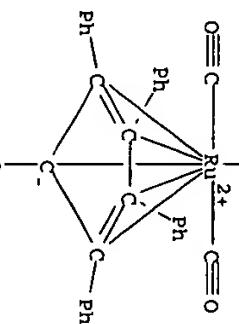
RL: RCT (Reactant); RACT (Reactant or reagent)

(*Candida antarctica* lipase can form anti-Kazlauskas acetylation

products of 2,4-pentanediol and 2,5-hexanediol)

RN 104439-77-2 CAPLUS

CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-eta.]-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][1,2,3,4,5-eta.]-1-hydroxy-2,3,4,5-tetraphenyl-1,2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)



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IT 9001-62-1

RL: CAT (Catalyst use); USES (Uses)

(Lipase B: *Candida antarctica* lipase can form anti-Kazlauskas acetylation products of 2,4-pentanediol and 2,5-hexanediol)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE *** THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 20 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:76732 CAPLUS
DOCUMENT NUMBER: 138:137021

TITLE: Process for the racemization of secondary alcohols using ruthenium compounds and chelating agents

INVENTOR(S): Riermeier, Thomas; Gross, Peter; Hoff, Manfred; Monsees, Axel; Dingerdissen, Uwe

PATENT ASSIGNEE(S): Degussa AG, Germany

SOURCE: PCT Int. Appl., 22 pp.
CODEN: PIXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003008361	Al	20030130	WO 2002-EP7743	20020711

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CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,

GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,

LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,

PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TZ, RU,

UG, US, UZ, VN, YU, ZA, ZM, AM, AZ, BY, KG, KZ, MD, RU,

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PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,

NE, SN, TD, TG DE 10133783 A1 20030206 DE 2001-10133783 20010716

PRIORITY APPLN. INFO.: MARPAT 138:137021 DE 2001-10133783 A 20010716

OTHER SOURCE(S):

AB A process for the racemization of secondary alcs. uses a mixt. of Ru precursor with N-toreq.1 chelating N-donor ligands or a complex comprising Ru and .gtoreq.1 chelating N-donor ligand. Thus, (+)-1-phenylethanol, N,N,N',N'-tetramethyl-1,3-propanediamine, and di-.mu.-chlorobis[(p-cymene)chlororuthenium(II)] were heated in PhMe at

PAGE 2-A

80. degree. in a Schlenk tube for 5 h to give a product having 1% enantiomeric excess. The process was also carried out simultaneously with a kinetic enzymic resoln.

IT

9001-62-1, Chirazyme L-2

RL: CAT (Catalyst use); USES (USES)

(dynamic kinetic resoln. of secondary alcs. using ruthenium

comps. and chelating agents)

RN

9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 37366-09-9, Benzeneruthenium(II) chloride dimer 52462-29-0

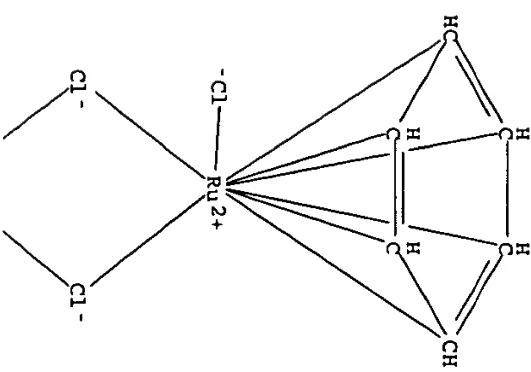
134524-84-8
RL: CAT (Catalyst use); USES (USES)

(process for the racemization of secondary alcs. using ruthenium

comps. and chelating agents)

RN

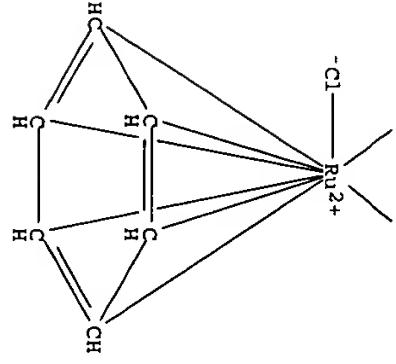
37366-09-9 CAPLUS
CN Ruthenium, bis(.eta.6-benzene)di-.mu.-chlorodichlorodi- (9CI) (CA INDEX NAME)



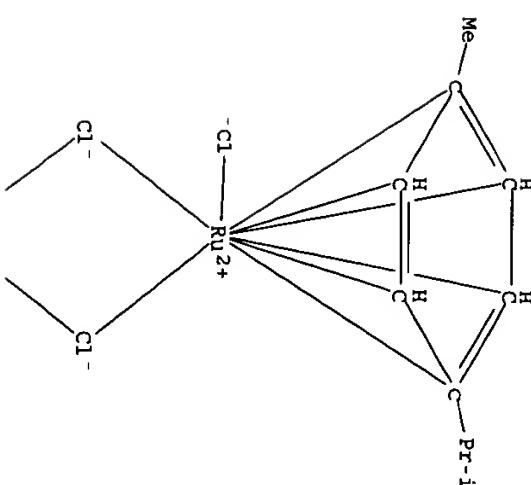
PAGE 1-A

RN

52462-29-0 CAPLUS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)

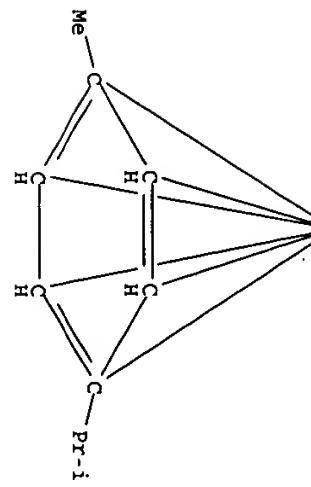
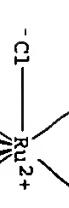


PAGE 1-A



PAGE 2-A

PAGE 2-A



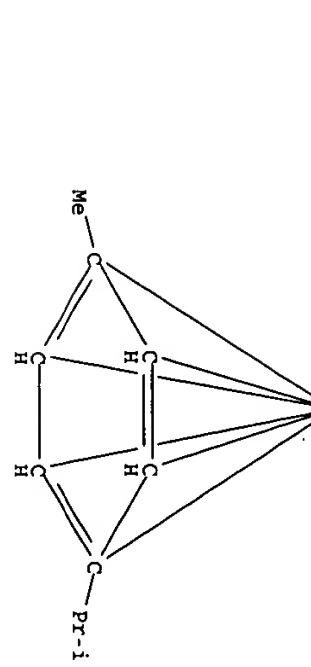
RN 134524-84-8 CAPLUS
Ruthenium, [(1,1'-binaphthalene)-2',2'-diylbis[diphenylphosphine-.kappa.P]]dichloro-, [SP-4-2-(S)]- (9CI) (CA INDEX NAME)

IT 9001-62-1, Lipase
RL: CAT (Catalyst use); USES (uses)
(pseudomonas sp.; chemoenzymic dynamic kinetic resoln. of
.beta.-halo alcs. and subsequent conversion of intermediate acetates to
chiral epoxides)
RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 104439-77-2
RL: CAT (Catalyst use); USES (uses)
(racemization catalyst; chemoenzymic dynamic kinetic
resoln. of .beta.-halo alcs. and subsequent conversion of
intermediate acetates to chiral epoxides)
RN 104439-77-2 CAPLUS
Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5-.eta.)-1-hydroxylato-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-.eta.)-1-hydroxy-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

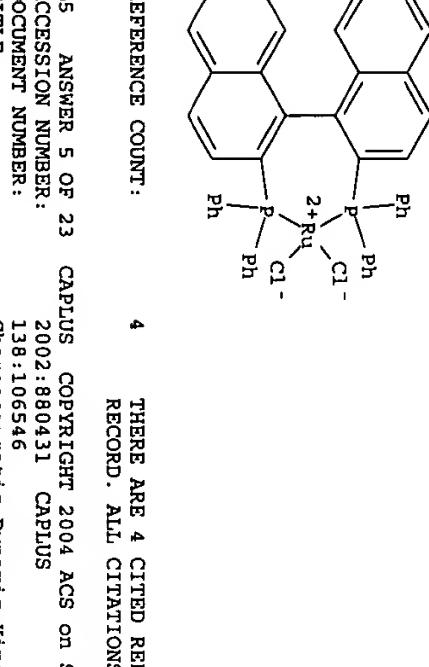
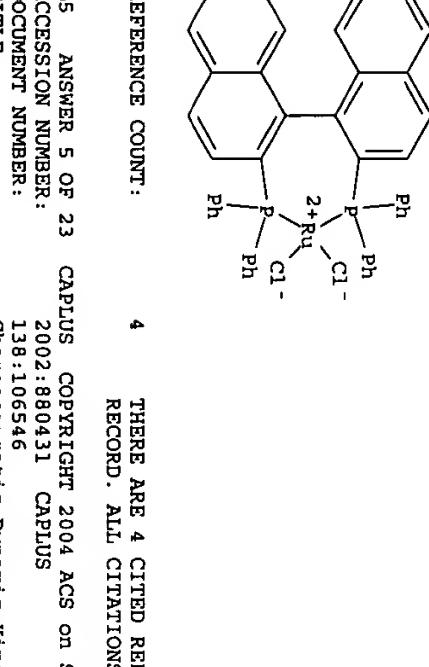
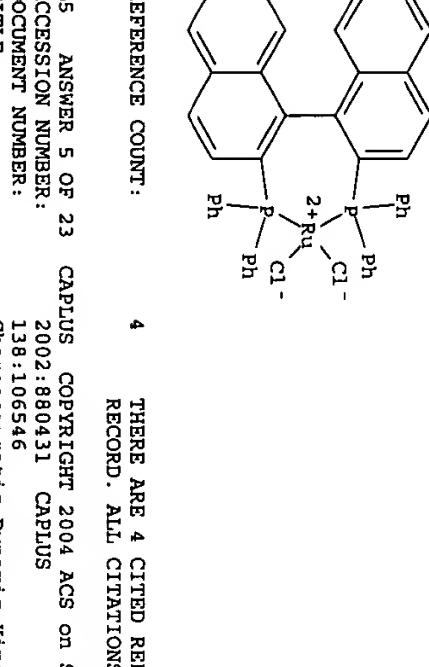
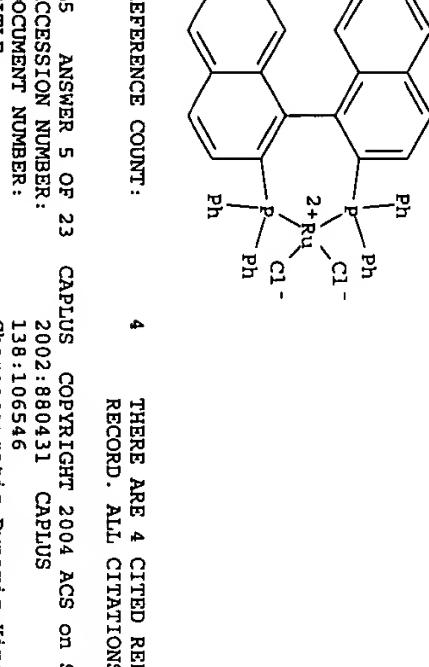
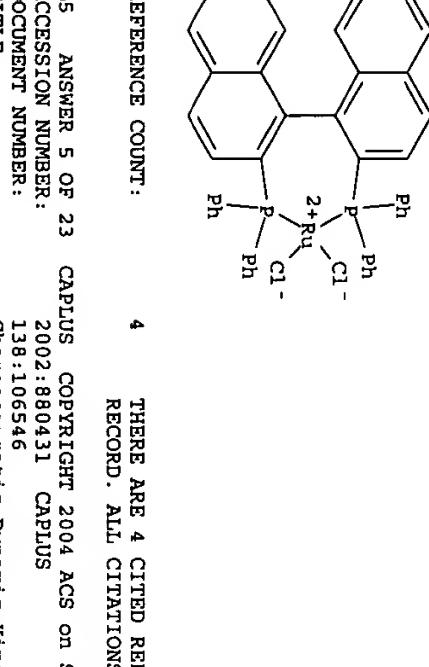
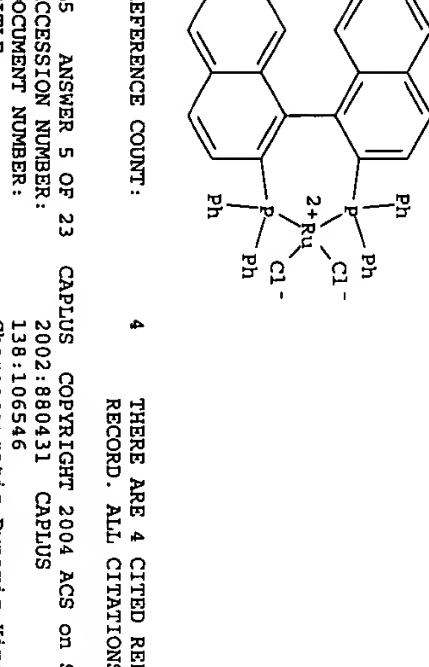
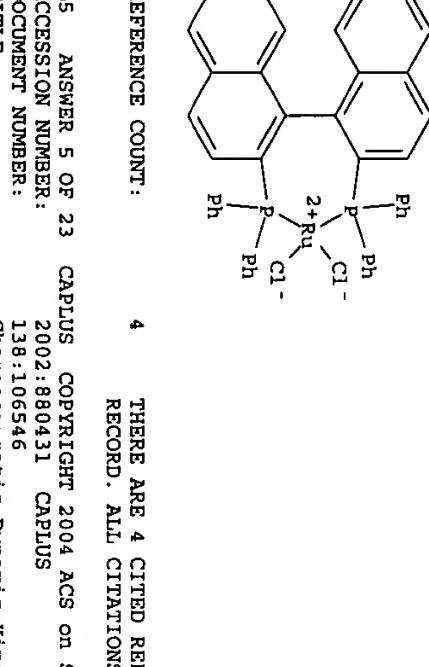
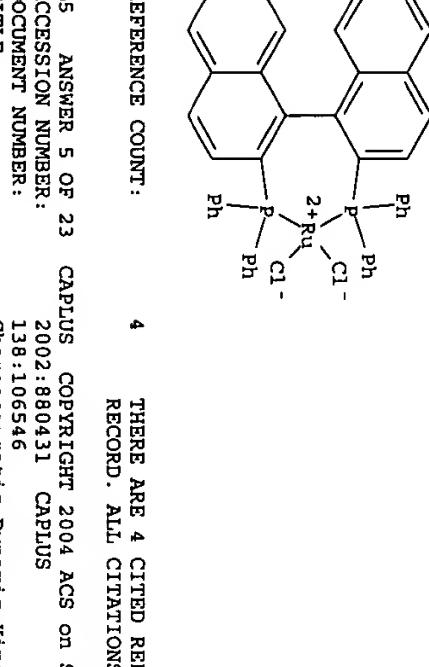
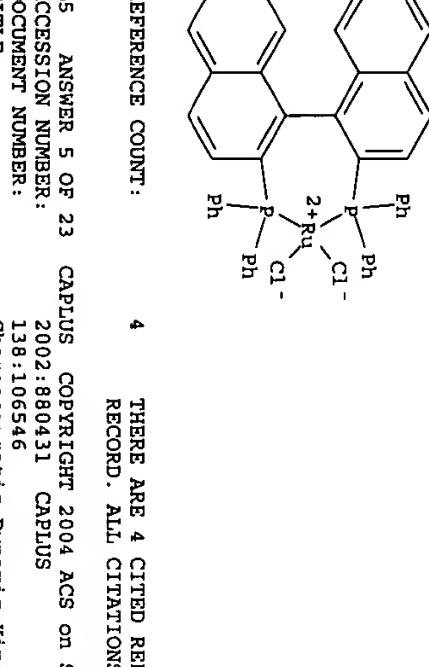
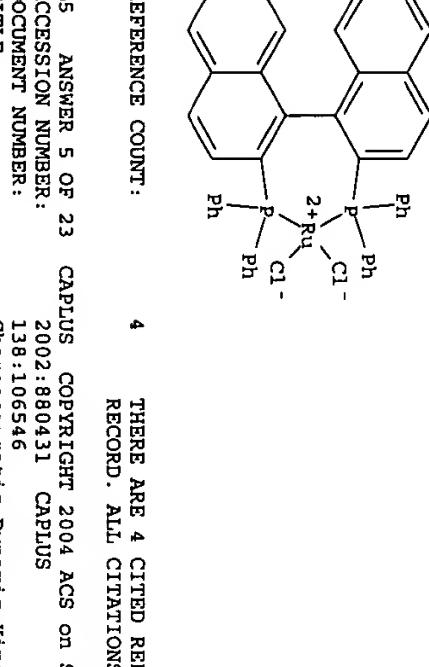
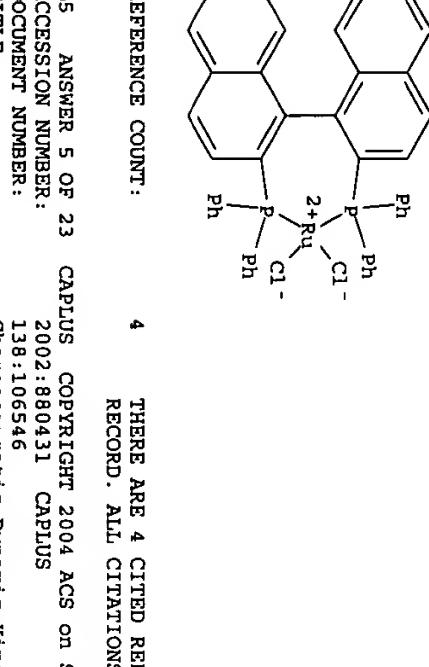
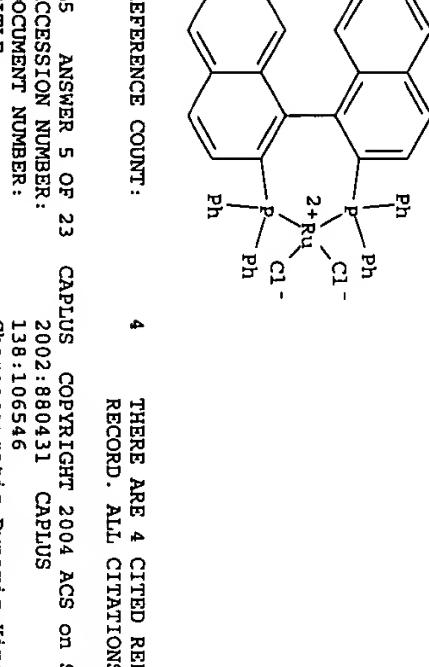
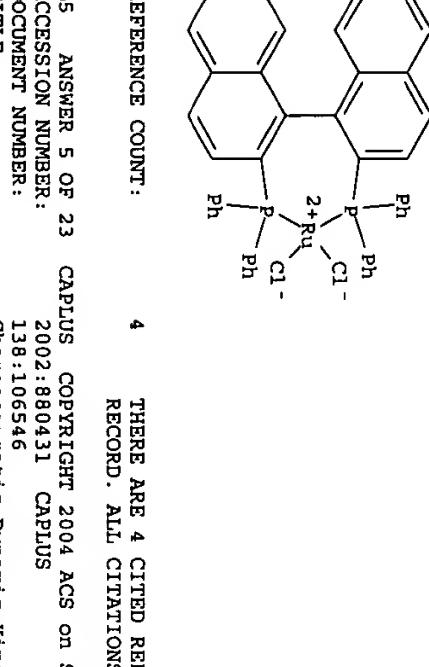
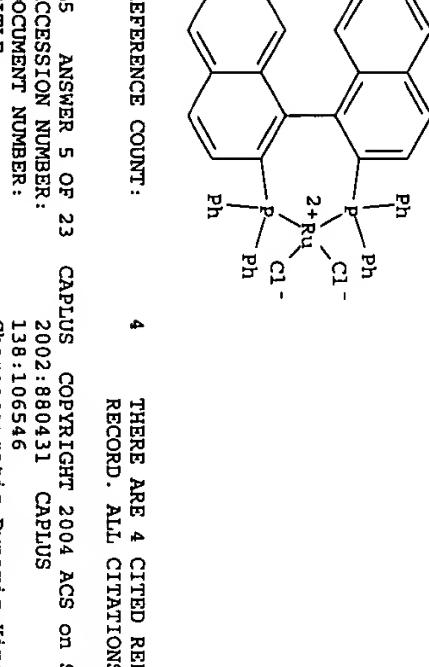
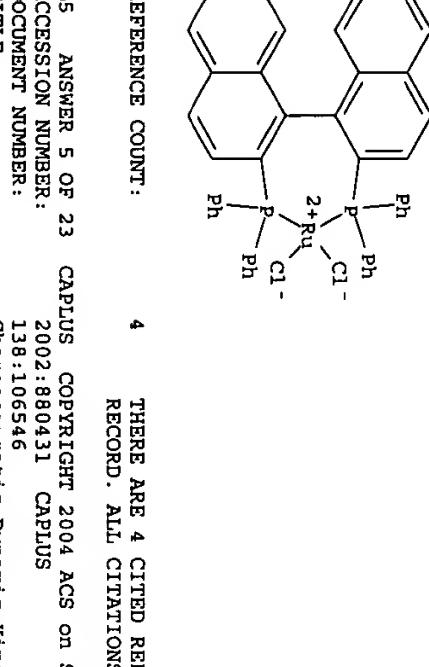
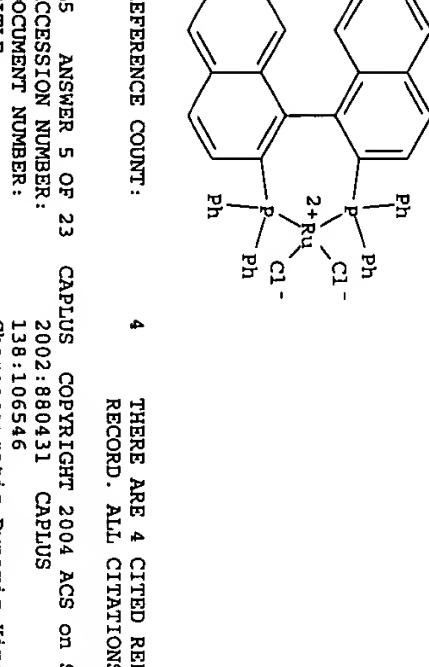
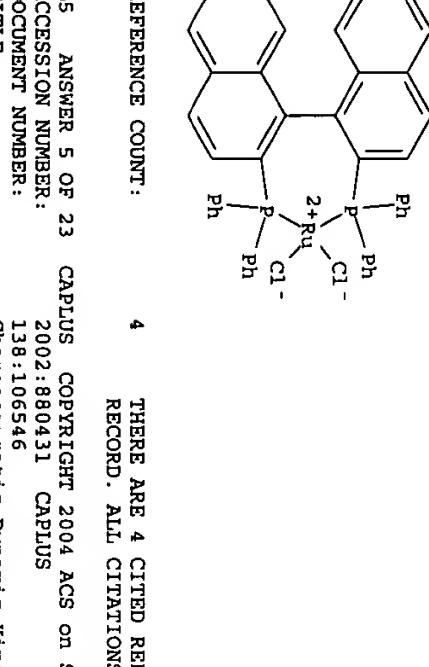
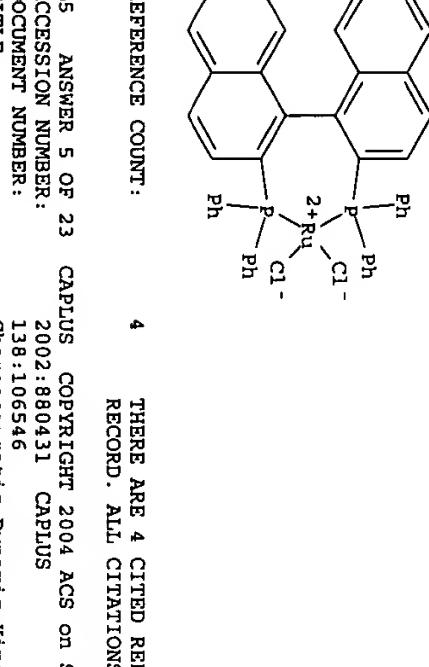
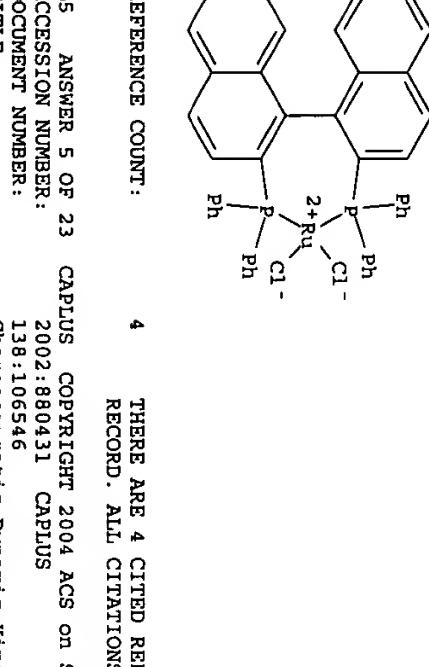
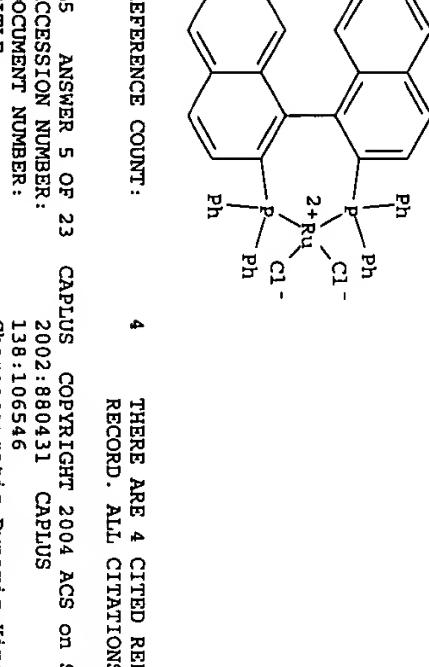
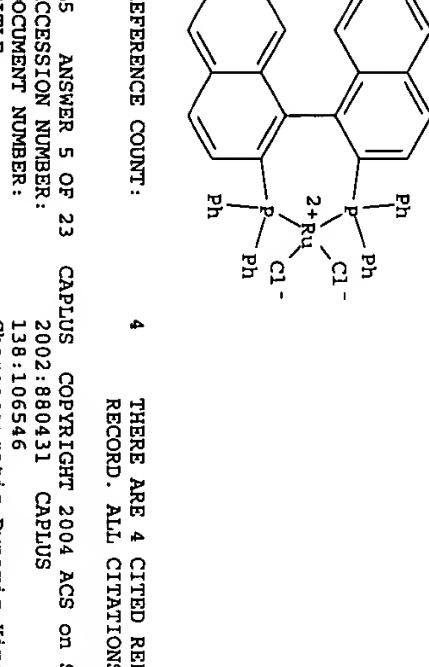
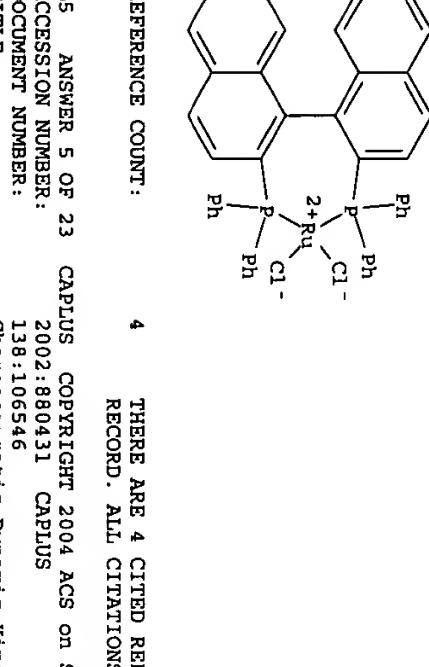
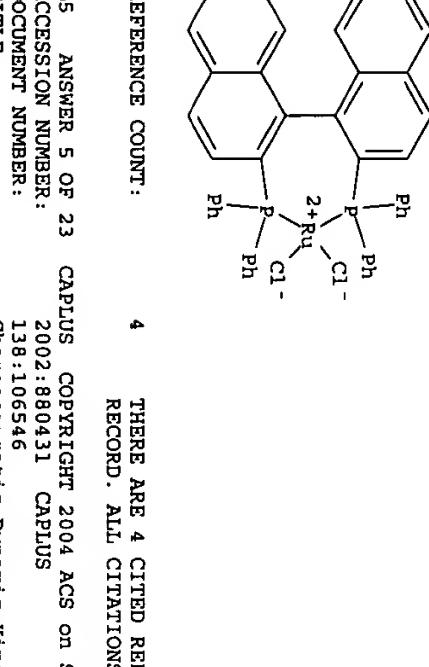
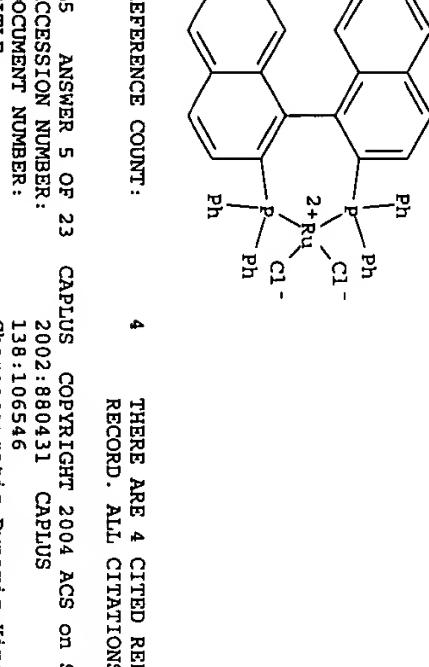
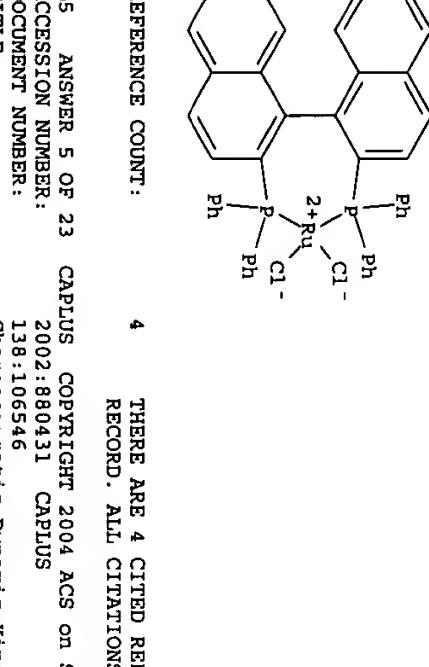
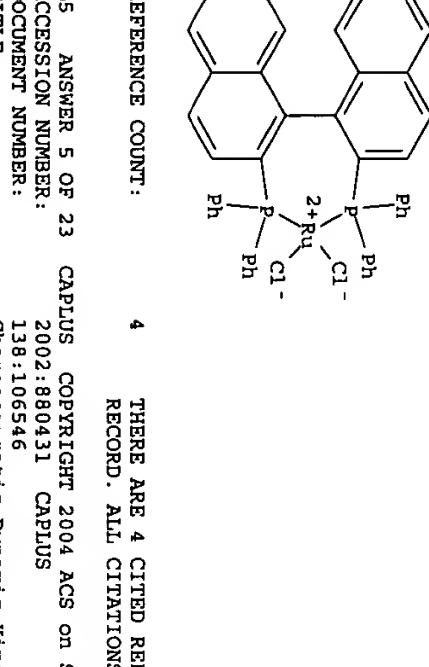
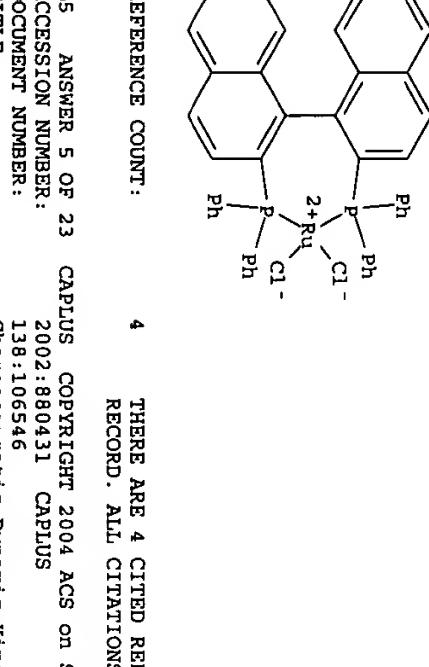
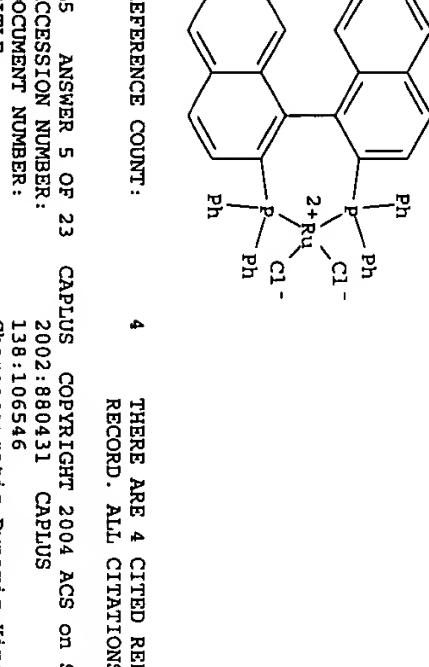
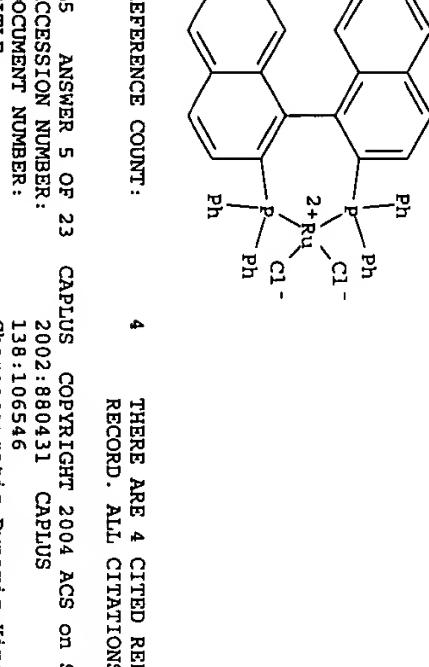
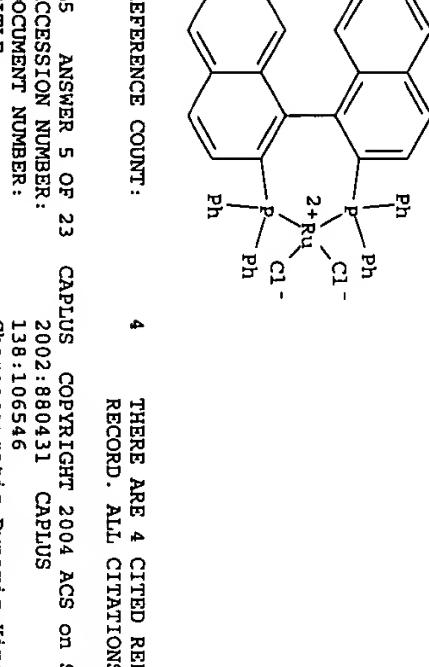
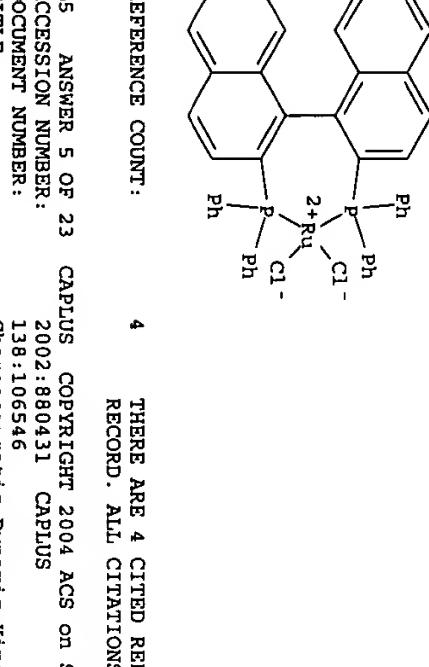
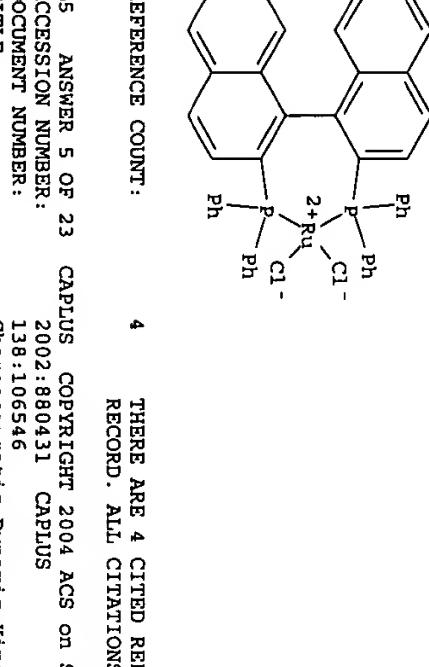
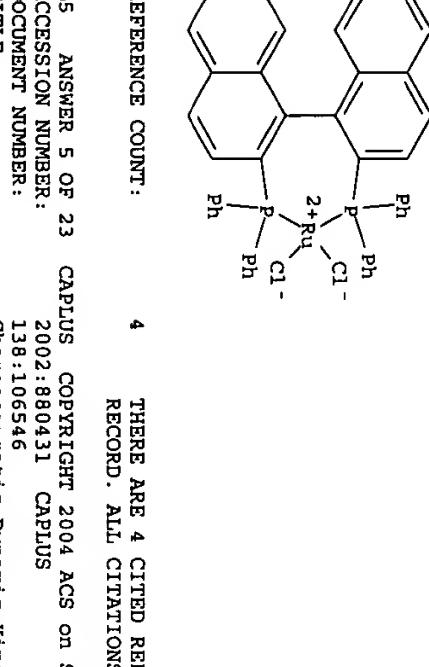
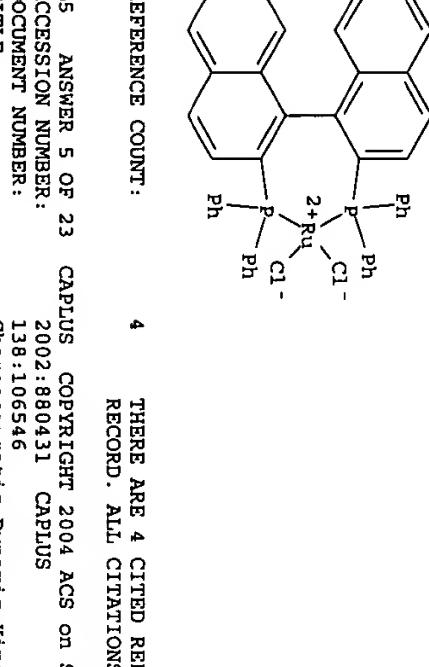
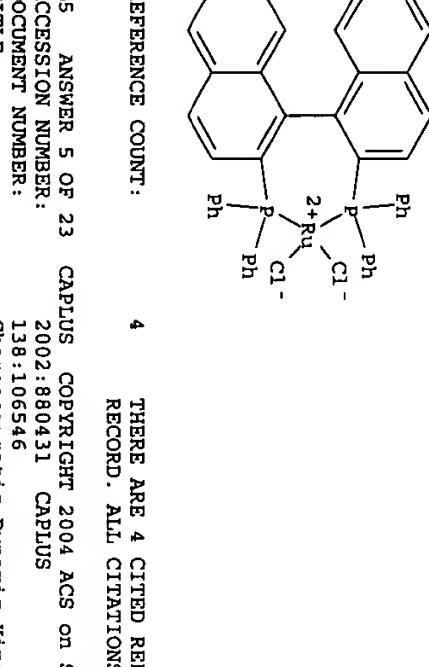
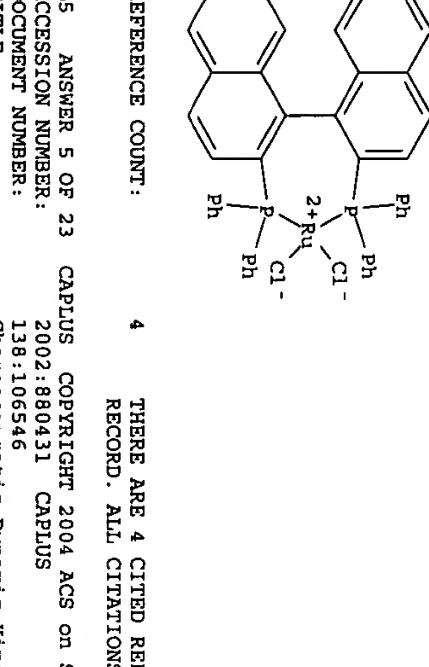
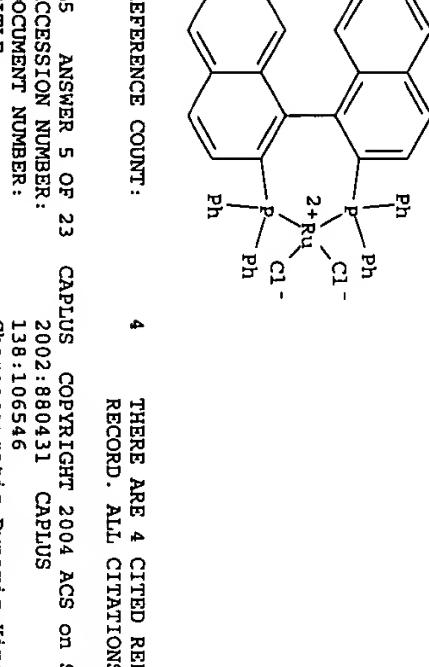
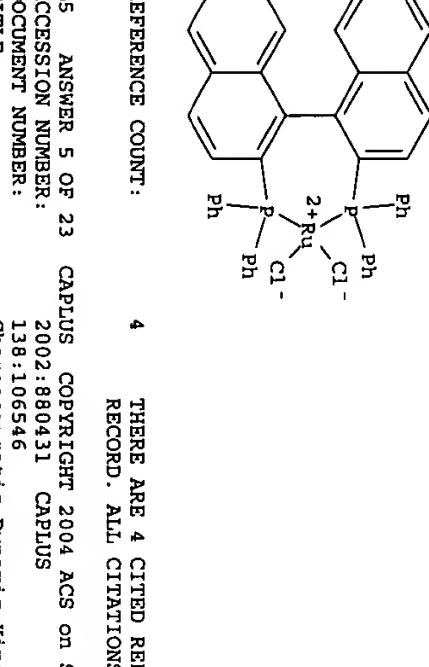
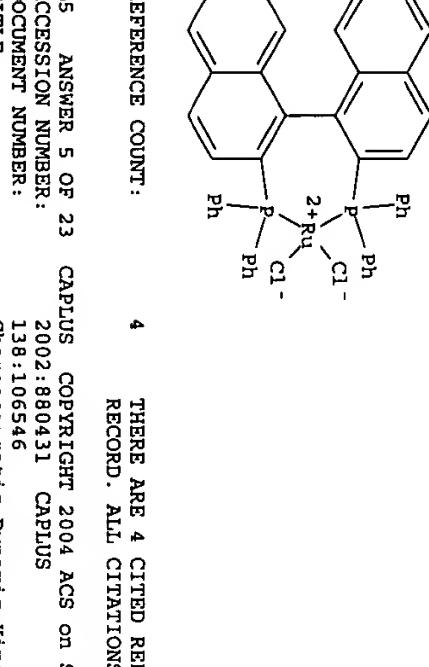
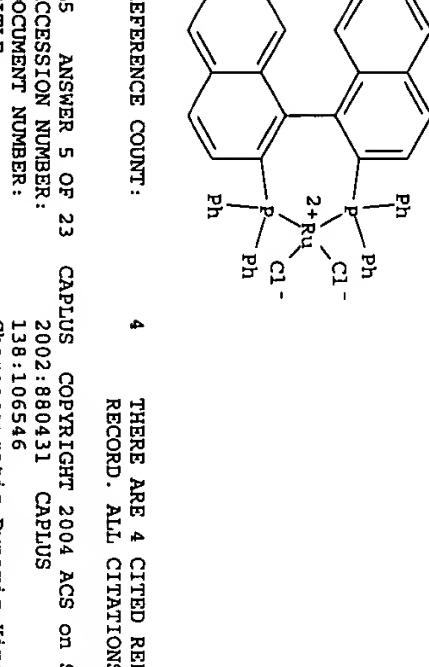
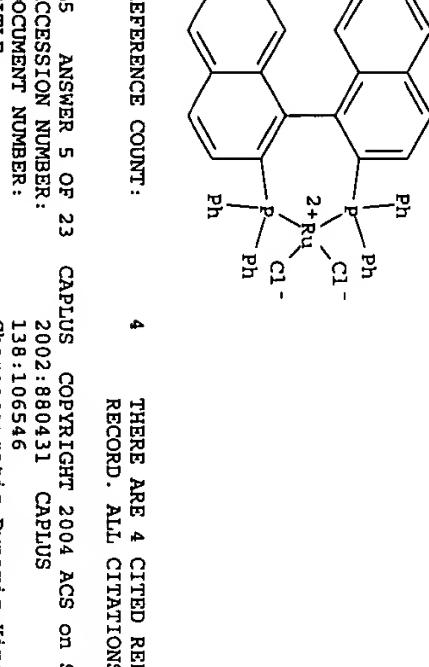
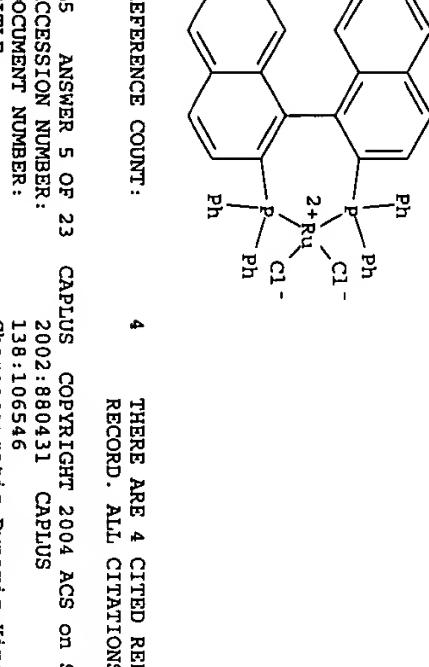
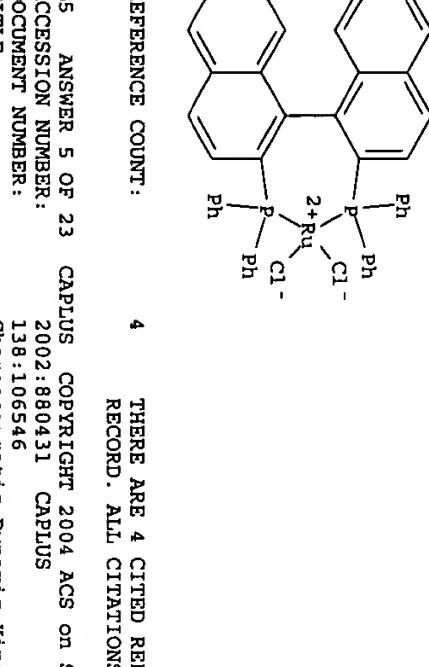
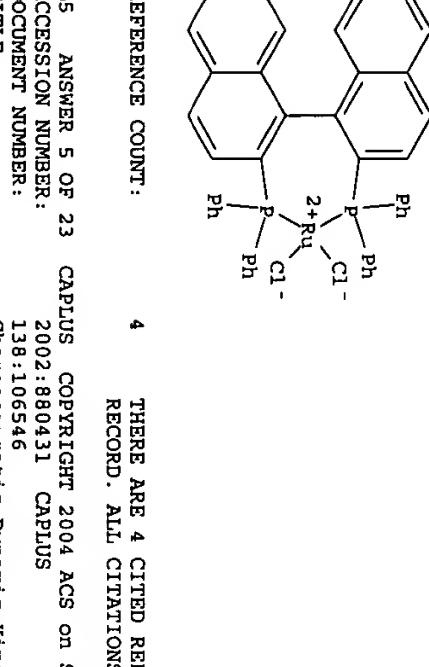
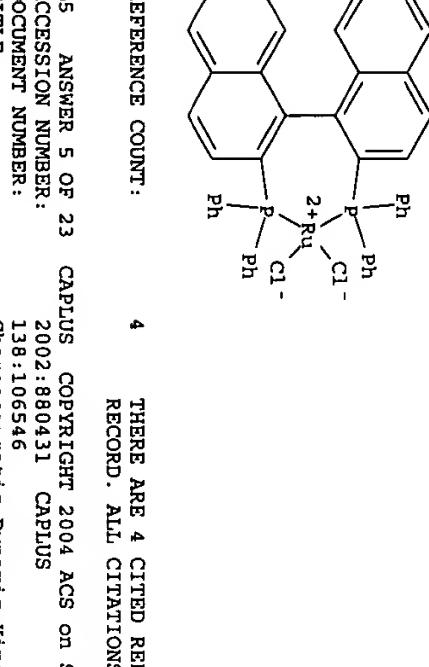
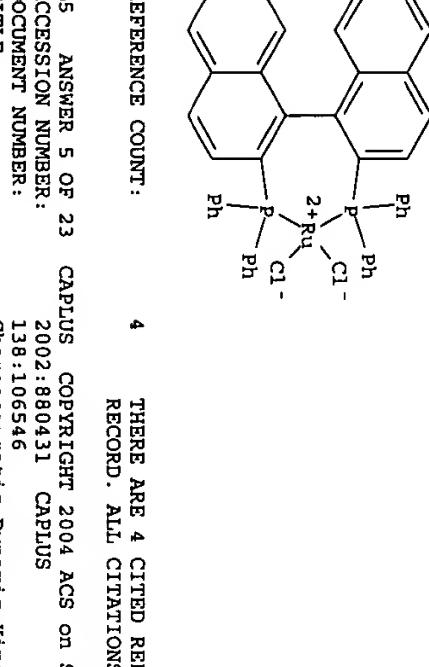
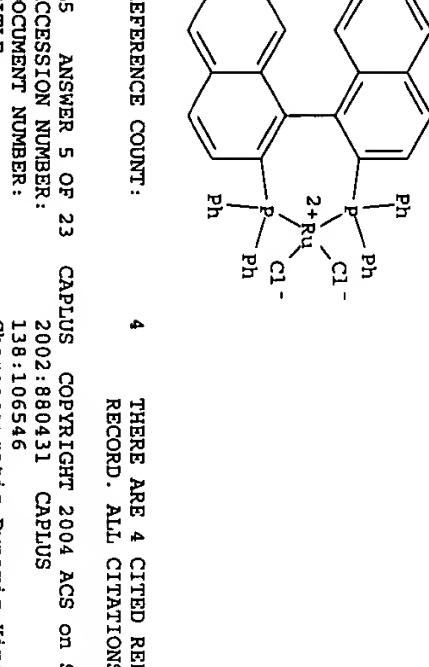
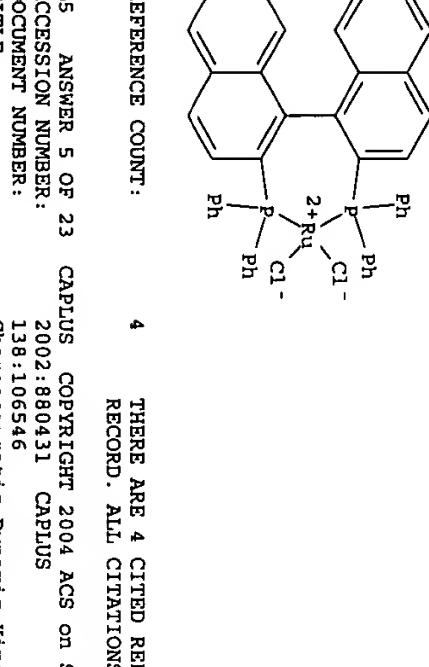
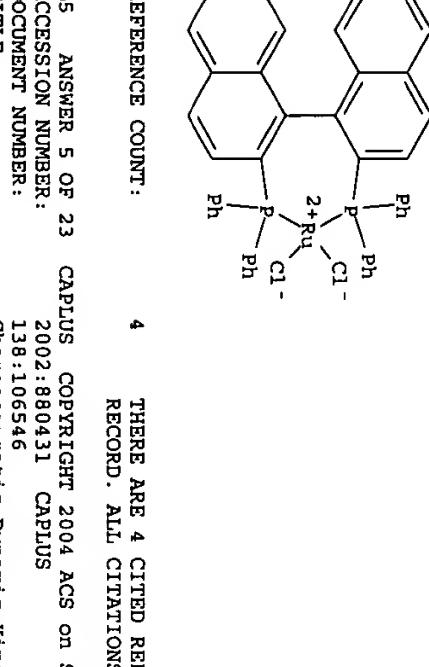
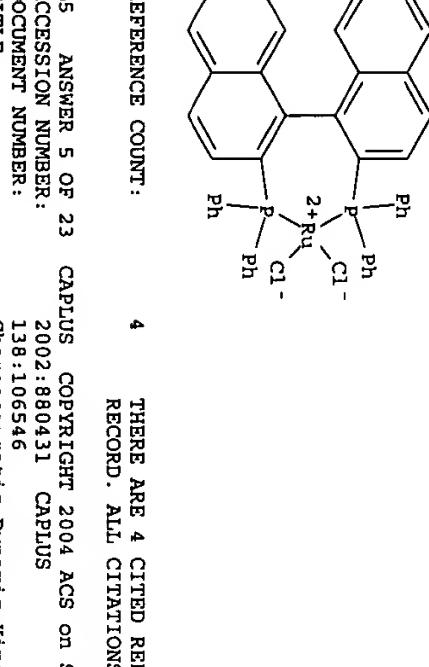
PAGE 1-A



RN 134524-84-8 CAPLUS
Ruthenium, [(1,1'-binaphthalene)-2',2'-diylbis[diphenylphosphine-.kappa.P]]dichloro-, [SP-4-2-(S)]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:880431 CAPLUS
DOCUMENT NUMBER: 138:106546
TITLE: Chemoenzymatic Dynamic Kinetic Resolution of .beta.-Halo Alcohols. An Efficient Route to Chiral Epoxides
AUTHOR(S): Pamies, Oscar; Baekvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-10691, Swed.
SOURCE: Journal of Organic Chemistry (2002), 67(25), 9006-9010
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE (S): CASREACT 138:106546
AB Enzymic resoln. of .beta.-chloro alcs. in combination with ruthenium-catalyzed alc. isomerization led to a successful dynamic kinetic resoln. (conversion up to 99% and ee up to 97%). The efficiency of the DKR is dramatically reduced when .beta.-bromo alcs. are used. The presence of the bromo substituent causes decomprn. of the ruthenium catalysts, which triggers the progressive deactivation of the enzyme. The synthetic utility of this procedure has been illustrated by the practical synthesis of different chiral epoxides.



REFERENCE COUNT:

43

THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 1-A

L5 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:858574 CAPLUS
DOCUMENT NUMBER: 138:271003
TITLE: Efficient lipase-catalyzed kinetic resolution of and dynamic kinetic resolution of .beta.-hydroxy nitriles. Correction of absolute configuration and transformation to chiral .beta.-hydroxy acids and .gamma.-amino alcohols

AUTHOR(S): Pamies, Oscar; Backvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, 106 91, Swed.
SOURCE: Advanced Synthesis & Catalysis (2002), 344(9), 947-952
CODEN: ASCAFT; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE (S): CASREACT 138:271003

AB Chemoenzymic dynamic kinetic resoln. of .beta.-hydroxy nitriles has been carried out using *Candida antarctica* lipase B and a ruthenium catalyst. The use of a hydrogen source to depress ketone formation in the dynamic kinetic resoln. yields the acetates in good yield and high enantioselectivity. It is shown that the ruthenium catalyst and the enzyme can be recycled when used in sep. reactions. Enantiomerically pure .beta.-hydroxy acid derivs. and .gamma.-amino alcs. were prep. from the hydroxy nitriles and acetates. The latter compds. were also used to establish the correct abs. configuration of the hydroxy nitriles and acetates.

IT

9001-62-1

RL: CAT (Catalyst use); USES (Uses)

(Lipase B; lipase-catalyzed kinetic resoln. and dynamic kinetic resoln. of .beta.-hydroxy nitriles and conversion to chiral .beta.-hydroxy acids and .gamma.-amino alcs.)

RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

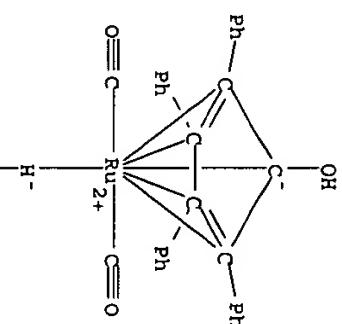
IT 104439-77-2

RL: CAT (Catalyst use); USES (Uses)

(lipase-catalyzed kinetic resoln. and dynamic kinetic resoln. of .beta.-hydroxy nitriles and conversion to chiral .beta.-hydroxy acids and .gamma.-amino alcs.)

RN 104439-77-2 CAPLUS

CN Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5-.eta.)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)



PAGE 2-A

IT

9001-62-1

RL: CAT (Catalyst use); USES (Uses)

(Lipase B; lipase-catalyzed kinetic resoln. and dynamic kinetic resoln. of .beta.-hydroxy nitriles and conversion to chiral .beta.-hydroxy acids and .gamma.-amino alcs.)

RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 104439-77-2

RL: CAT (Catalyst use); USES (Uses)

(lipase-catalyzed kinetic resoln. and dynamic kinetic resoln. of .beta.-hydroxy nitriles and conversion to chiral .beta.-hydroxy acids and .gamma.-amino alcs.)

RN 104439-77-2 CAPLUS

CN Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5-.eta.)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

IT

137:384594

L5 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:456611 CAPLUS
DOCUMENT NUMBER: 137:384594
TITLE: An efficient and mild ruthenium-catalyzed racemization of amines: application to the synthesis of enantiomerically pure amines

AUTHOR(S): Pamies, Oscar; Ell, Alida H.; Samec, Joseph S. M.; Hermans, Nina; Backvall, Jan-E.
CORPORATE SOURCE: Arrhenius Laboratory, Department of Organic Chemistry, Stockholm University, Stockholm, SE-10691, Swed.
SOURCE: Tetrahedron Letters (2002), 43(26), 4699-4702
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An efficient and mild Ru-catalyzed racemization of amines under

transfer hydrogenation conditions is reported. A significant advantage of this new procedure is that the ruthenium hydrogen transfer catalysts allow high functional group tolerance. Interestingly, both primary and secondary amines were efficiently racemized under these conditions. We also report on the combination of this new amine racemization with an enzymic kinetic resoln. of primary amines.

IT 9001-62-1, Lipase 104439-77-2

RL: CAT (Catalyst use); USES (Uses)

(ruthenium-catalyzed racemization of amines and subsequent

lipase-catalyzed kinetic resoln.)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS

CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.)-1-hydroxylato-

2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl] [(1,2,3,4,5-.eta.)-1-hydroxy-

2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl] di- (9CI) (CA INDEX NAME)

PAGE 1-A

SOURCE:

Tetrahedron: Asymmetry (2002), 13(8), 879-884

CODEN: TASYE3; ISSN: 0957-4166

BL, Neth. Journal

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Three new ruthenium-based catalytic systems are described which are capable of catalyzing the racemization of chiral secondary alcs.

In addn., one of these systems, [TosN(CH₂)₂RuCl(p-cymene)]/TEMPO, was able to catalyze the in situ racemization during enzymic

resoln., i.e. dynamic kinetic resoln.

IT 9001-62-1, Novozym 435

RL: NUU (Other use, unclassified); USES (Uses)

(additive; effect of additives on racemization of secondary alcs. in presence of ruthenium compds./TEMPO catalytic systems)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 52462-29-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(efficient ruthenium compds./TEMPO catalytic systems for

racemization of secondary alcs. and potential applications to

dynamic kinetic resoln.)

RN 52462-29-0 CAPLUS

CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-

methyl)benzene]di- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

34

THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:403138 CAPLUS
DOCUMENT NUMBER: 137:369562

TITLE: Efficient ruthenium-catalyzed racemization of secondary alcohols: application to dynamic kinetic resolution

Dijksman, Arne; Elzinga, Joffrey M.; Li, Yu-Xin; Arends, Isabel W. C. E.; Sheldon, Roger A.

Department of Biotechnology, Biocatalysis and Organic Chemistry, Delft University of Technology, Delft, 2628

BL, Neth. Tetrahedron: Asymmetry (2002), 13(8), 879-884

CODEN: TASYE3; ISSN: 0957-4166

Journal

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Three new ruthenium-based catalytic systems are described which are capable of catalyzing the racemization of chiral secondary alcs.

In addn., one of these systems, [TosN(CH₂)₂RuCl(p-cymene)]/TEMPO, was able to catalyze the in situ racemization during enzymic

resoln., i.e. dynamic kinetic resoln.

IT 9001-62-1, Novozym 435

RL: NUU (Other use, unclassified); USES (Uses)

(additive; effect of additives on racemization of secondary alcs. in presence of ruthenium compds./TEMPO catalytic systems)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 52462-29-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(efficient ruthenium compds./TEMPO catalytic systems for

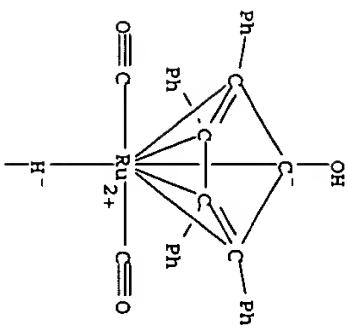
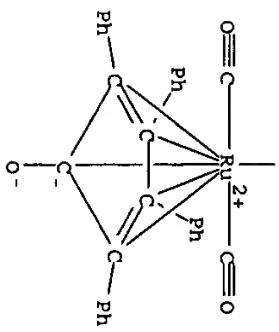
racemization of secondary alcs. and potential applications to

dynamic kinetic resoln.)

RN 52462-29-0 CAPLUS

CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-

methyl)benzene]di- (9CI) (CA INDEX NAME)



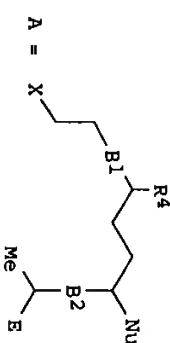
PAGE 2-A

DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

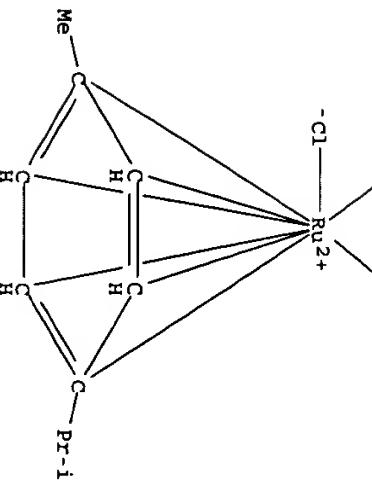
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002032844	A2	20020425	WO 2001-EP11992	20011016
WO 2002032844	C1	20030821		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10051136	A1	20020418	DE 2000-10051136	20001016
DE 10134172	A1	20030123	DE 2001-10134172	20010713
AU 200201693	A5	20020429	AU 2002-21693	20011016
EP 1358144	A1	20031105	EP 2001-987736	20011016
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRIORITY APPLN. INFO.:			DE 2000-10051136 A	20001016
			DE 2001-10134172 A	20010713
WO 2001-EP11992	W	20011016		

OTHER SOURCE (S): CASREACT 136:340534; MARPAT 136:340534

GI



AB The invention relates to **racemic** and esp. **non-racemic** acyloins, $\text{R}_1\text{C}(\text{O})\text{CH}_2\text{OH}$ [I; $\text{R}_1 = \text{H}$, alkyl (esp. Me, Et, Pr), aryl, alkylaryl, $\text{CH}_2\text{-aryl}$, $(\text{CH}_2)_2\text{-aryl}$, vinyl, alkyne, propynyl, allyl, 3,3-dialkylallyl, $\text{C}_3\text{-7-cycloalkyl}$, $\text{CHnF}_3\text{-n}$, $\text{C}_3\text{-7-oxacycloalkyl}$; $\text{R}_2 =$ alkyl, aryl, alkylaryl, $\text{CH}_2\text{-aryl}$, $(\text{CH}_2)_2\text{-aryl}$, vinyl, alkyne, propynyl, allyl, 3,3-dialkylallyl, E- or Z-haloalkenyl, 3,3-dihaloallyl, $\text{C}_3\text{-7-cycloalkyl}$, $\text{CHnF}_3\text{-n}$, $\text{C}_3\text{-7-oxacycloalkyl}$, alkylpropynyl, 1-alkylallyl, 3,3-dialkylallyl A (joined at X); $\text{B}_1, \text{B}_2 =$ single or E-, Z-, E/Z-double bond; $\text{B}_1 =$ epoxide; $\text{R}_4 = \text{H}$, F, Cl, Br, I, alkyl (esp. Me, Et, $\text{CHnF}_3\text{-n}$), aryl, alkylaryl, $\text{CH}_2\text{-aryl}$, $(\text{CH}_2)_2\text{-aryl}$, vinyl, alkyne, propynyl, allyl, 3,3-dialkylallyl, $\text{C}_3\text{-7-oxacycloalkyl}$, $\text{CHnF}_3\text{-n}$, $\text{C}_3\text{-7-oxacycloalkyl}$; $\text{E} = \text{Me}$, CH_2OH , $\text{CH}_2\text{-PG}$, CHO , $\text{CO}_2\text{-PG}$, $\text{CH}_2\text{-halo}$, CONR_2 , $\text{CON}(\text{PG})_2$, $\text{CON}(\text{OMe})\text{Me}$, CN; $\text{R} =$ alkyl; $\text{Nu} = \text{R}_4$, O-PG, OR, N(PG)₂, N(alkyl)₂, S-PG, S-alkyl, Se-alkyl, CN, NS, aryl, heteroaryl; PG = protective group], their derivs., a method for the prodn. thereof and the use of the same for producing epothilones and their derivs. The invention esp. relates to the prodn. of acyloins in a non-racemic form by means of diastereomer sepn. or synthesis using auxiliary agents and by means of enzymic resoln. of racemates. The invention also relates to epothilone synthesis components, a method for the prodn. thereof and the use of synthesis components for producing epothilones and



REFERENCE COUNT: 31

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2002;314889 CAPLUS
 DOCUMENT NUMBER: 136:340534
 TITLE: Method for the production of asymmetrically substituted acyloins and derivatives and for the production of epothilones B, D and their derivatives
 INVENTOR (S): Wessjohann, Ludger A.; Scheid, Guenther; Bornscheuer, Uwe; Henke, Erik; Kuit, Wouter; Orru, Romano
 PATENT ASSIGNEE (S): Morphochem A-G, Germany
 SOURCE: PCT Int. Appl., 182 pp.
 CODEN: PIXXD2

their derivs. Thus, optically active (Z)-3-hydroxy-6,10-dimethyl-11-[(tert-butyldimethylsilyl)oxy]undeca-5,9-dien-2-one was prep. from (+)-(-)-Z)-3-acetoxyl-10-dimethyl-11-[(tert-butyldimethylsilyl)oxy]undeca-5,9-dien-2-one via enzymic resoln. with Chirazyme L6. The optically active hydroxy ketone was converted to three 3-O-(tert-butyldimethylsilyl)epothilone D stereoisomers.

IT 104621-48-9

RL: CAT (Catalyst use); USES (uses)
(prep. of asym. substituted acyloins and derivs. for the of epothilone B, D and their derivs.)

RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 9016-18-6 CAPLUS
CN Esterase, carboxyl (8CI, 9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104621-48-9 CAPLUS
CN Ruthenium, bis(acetato- κ O, κ O')[(1R)-[1,1'-binaphthalene]-2,2'-diyl]bis[diphenylphosphine- κ P]-, (OC-6-22-.DELTA.)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104621-48-9 CAPLUS
CN Ruthenium, bis(acetato- κ O, κ O')[(1R)-[1,1'-binaphthalene]-2,2'-diyl]bis[diphenylphosphine- κ P]-, (OC-6-22-.DELTA.)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

15 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:255775 CAPLUS
DOCUMENT NUMBER: 137:278899

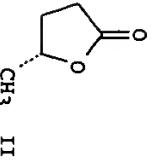
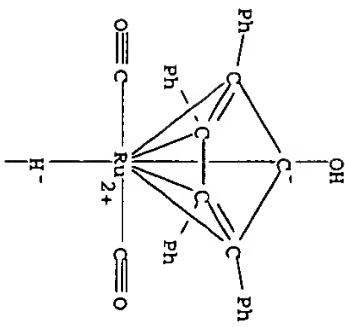
TITLE: Dynamic kinetic resolution of
.gamma.-hydroxy acid derivatives

AUTHOR(S): Ruoho, Ann-Britt L.; Pamies, Oscar; Faber, Kurt;
Arrhenius Laboratory, Department of Organic Chemistry,
Stockholm University, Stockholm, SE-10691, Swed.

CORPORATE SOURCE: Tetrahedron Letters (2002), 43(16), 2983-2986

SOURCE: CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE (S): CASREACT 137:278899
GI

PAGE 1-A



PAGE 2-A

AB .gamma.-Hydroxy acid derivs. MeCH(OAc)CH2CH2C(=O)R1 [R = H; R1 = Me3CO,

[Me2CH]2N] (I) undergo enzymic kinetic resoln. with 4-chlorophenyl acetate in toluene in the presence of *Pseudomonas cepacia* lipase to give nonracemic I (R = Ac) in 44-56% yields and in 77-99% ee. When the enzymic resoln. is performed under anaerobic conditions in the presence of a bis(hydroxycyclopentadienyl)diruthenium tetracarbonyl hydride racemization catalyst and in the presence of 2,4-dimethyl-3-pentanol as a hydride donor, nonracemic I (R = Ac) is isolated in 43-93% yields and in 71-98% ee from the dynamic kinetic resoln. MeCH(OAc)CH2CH2C(=O)(CHMe2)2, prep. in 93% yield and 98% ee from the dynamic kinetic resoln. of I [R = H; R1 =

(Me2CH)2N], undergoes hydrolysis with lithium hydroxide in methanol followed by acidic lactonization to give the nonracemic .gamma.-lactone II in 92% ee.

IT 9001-62-1, Lipase 104439-77-2

RL: CAT (Catalyst use); USES (uses)
(enantioselective prep. of .gamma.-hydroxy acid derivs. by either kinetic or dynamic kinetic resoln. of .gamma.-hydroxy acid derivs. with Pseudomonas cepacia lipase in absence or presence of ruthenium racemization catalyst)

RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

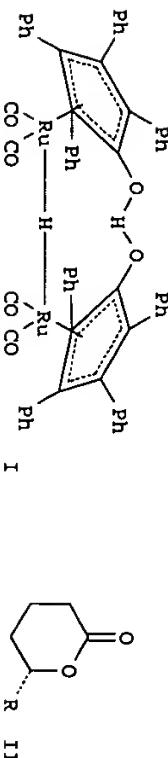
RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

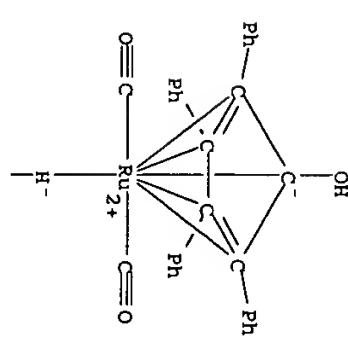
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMATTED

L5 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:64783 CAPLUS
DOCUMENT NUMBER: 136:263059
TITLE: Enzymatic kinetic resolution and
chemoenzymatic dynamic kinetic resolution of
.delta.-hydroxy esters. An efficient route to chiral
.delta.-lactones
AUTHOR(S): Pamies, Oscar; Baekvall, Jan-E.
CORPORATE SOURCE: Arrhenius Laborator, Department of Organic Chemistry,
Stockholm University, Stockholm, SE-106 91, swed.
SOURCE: Journal of Organic Chemistry (2002), 67(4), 1261-1265
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE (S): CASREACT 136:263059
GI



nonracemic .delta.-acetoxy esters (R) $-RCH(OAc)CH_2CH_2CH_2CO_2CMe_3$ (R = Me, Et) and the (S)-.delta.-hydroxy esters $RCH(OH)CH_2CH_2CH_2CO_2CMe_3$ (R = Et) in 98-99% ee (E value up to 360). When the Shvo ruthenium isomerization catalyst I was added to the enzymic acylation conditions, the combination of the enzymic kinetic **resoln.** with a ruthenium-catalyzed alc. racemization led to an efficient dynamic kinetic **resoln.** of the .delta.-hydroxy esters to give (R) $-RCH(OAc)CH_2CH_2CH_2CO_2CMe_3$ in 87-89% yields and in ee up to 99%. The .delta.-hydroxy esters were converted to .delta.-lactones II, important building blocks in the synthesis of natural products and biol. active compds., by deacetylation with lithium hydroxide in toluene/methanol followed by acidification with hydrochloric acid. (S)-5-(tert-butyldimethylsilyloxy)heptanal (S)- $EtCH(OTBDMSC_6H_4CH_2CH_2CHO$ ($TBDMS$ = tert-butyldimethylsilyl), a key intermediate in the syntheses of widely used com. insecticide Spinosyn A, was prep'd. from (S)- $EtCH(OH)CH_2CH_2CH_2CO_2CMe_3$ by silylation of the secondary alc. followed by redn. of the ester with disobutylaluminum

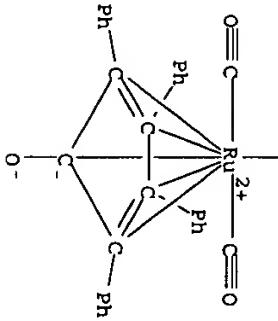


PAGE 2-A

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L5 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:868714 CAPLUS
DOCUMENT NUMBER: 136:4770
TITLE: Process for the preparation of enantiomerically
enriched esters and alcohols
INVENTOR(S): Verzijl, Gerardus Karel Maria; De Vries, Johannes
Gerardus; Broxterman, Quirinus Bernardus
PATENT ASSIGNEE(S): DSM N.V., Neth.

RL: CAT (Catalyst use); USES (Uses)
 (Pseudomonas cepacia; enantioselective prepn. of .delta.-lactones by
 dynamic kinetic resoln. of .delta.-hydroxy esters by
 acylation with 4-chlorophenyl acetate in presence of lipase and
 ruthenium isomerization catalyst)
 9001-62-1 CAPLUS
 Lipase, tracyclyglycerol (9CI) (CA INDEX NAME)
 *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
 IT 104439-77-2
 RL: CAT (Catalyst use); USES (Uses)
 (enantioselective prepn. of .delta.-lactones by dynamic kinetic



resoln. of delta.-hydroxy esters by acylation with
4-chlorophenyl acetate in presence of lipase and ruthenium
isomeric catalyst) (CA INDEX NAME)

AUTHOR (S): delta.-lactones
Pamies, Oscar; Baeckvall, Jan-E.
CORPORATE SOURCE: Arrhenius Laboratory, Department of Organic Chemistry,

SOURCE: Journal of Organic Chemistry (20)

DISCUSSION

PUBLISHER: AMERICAN CHEMICAL SOCIETY
DOCUMENT TYPE: Journal

DOCUMENT NUMBER: **00000000000000000000000000000000**

OTHER SOURCE(S) : CASREACT 136:263059

61

PAGE 1-M

LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090396	A1	20011129	WO 2001-NL383	20010521
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BE, BJ, CF, CG, CT, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
NL 1015313	C2	20011127	NL 2000-1015313	20000526
EP 1283898	A1	20030219	EP 2001-932412	20010521
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003533993	T2	20031118	JP 2001-586591	20010521
PRIORITY APPLN. INFO.:				
WO 2001-NL383	W	20010521	WO 2001-1015313	A

OTHER SOURCE(S): CASREACT 136:4770; MARPAT 136:4770

AB Method for the prepn. of an enantiomerically enriched ester, in which a mixt. of the enantiomers of the corresponding secondary alc. is subjected, in the presence of an acyl donor, to an enantioselective conversion in the presence of a racemization catalyst upon which the ester is formed and an acyl donor residue is obtained, and in which the acyl donor residue is irreversibly removed from the phase in which the enantioselective conversion is carried out enzymically and a transfer hydrogenation catalyst is used as racemization catalyst. The secondary alc. can be formed in situ from the corresponding ketone, in the presence of a H donor. It is also possible to use a mixt. of the secondary alc. and the corresponding ketone as substrate. Preferably the acyl donor is chosen so that the acyl donor residue is converted in situ into another compd. and/or the acyl donor residue is removed via distn. under reduced pressure. The enantiomerically enriched esters obtained can subsequently be converted into the corresponding enantiomerically enriched alcs., which are desirable intermediate products in the prepn. of liq. crystals, agro chems. or pharmaceuticals.

IT 9001-62-1, Novozyme 435 52462-29-0 104439-77-2

RL: CAT (Catalyst use); USES (USES)

(prep. of enantiomerically enriched esters and alcs.)

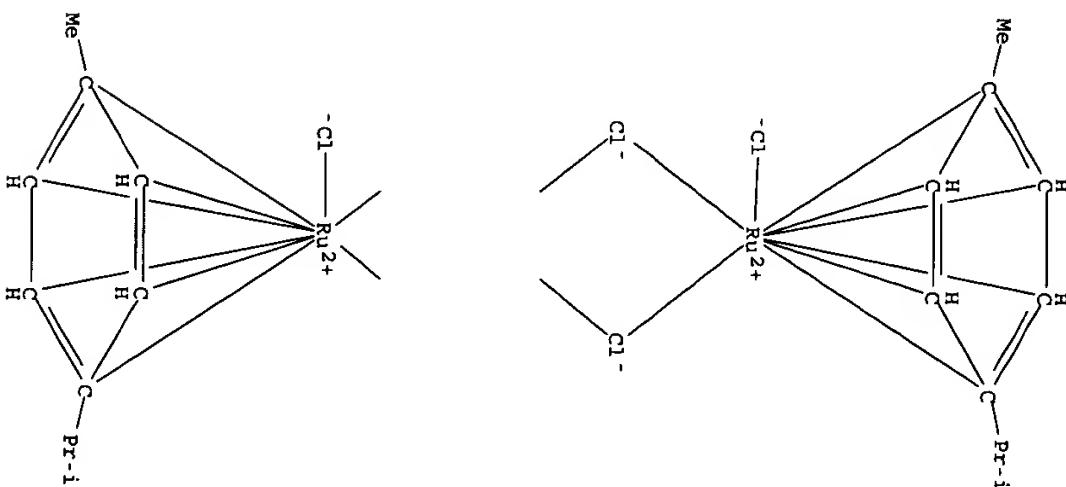
RN 9001-62-1 CAPIUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 52462-29-0 CAPIUS

CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,.eta.)-1-methyl-4-(1-methylethyl)benzenedi- (9CI) (CA INDEX NAME)



PAGE 2-A

RN 104439-77-2 CAPIUS
 CN Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5,.eta.)-1-hydroxylato-2,3',4',5'-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5,.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

PAGE 1-A

AB
An efficient kinetic **resoln.** of **racemic** .beta.-hydroxy nitriles was performed via *Candida antarctica* lipase (N-435)-catalyzed transesterification. A variety of **racemic** alkyl, aryl, and aryloxymethyl substituted .beta.-hydroxy nitriles was efficiently transformed to the corresponding enantiomerically pure acetates (ee >99% and conversion = 50%) with E values from 40 to >1000. The combination of the enzymic kinetic **resoln.** with a ruthenium-catalyzed alc. racemization led to a dynamic kinetic **resoln.** (ee's up to 99% yields up to 85%).

IT 9001-62-1, Lipase 104439-77-2

RL: CAT (Catalyst use); USES (Uses)

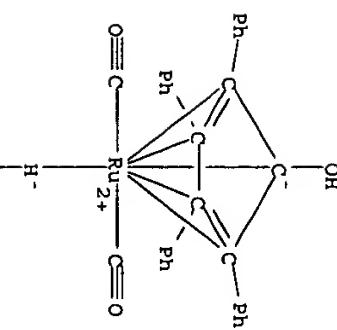
(lipase-catalyzed kinetic **resoln.** and dynamic kinetic

resoln. of .beta.-hydroxy nitriles)

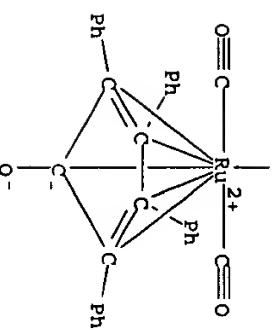
RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS
CN Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5-.eta.)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)



PAGE 2-A



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

15 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:669911 CAPLUS

DOCUMENT NUMBER:

TITLE: Efficient lipase-catalyzed kinetic resolution

and dynamic kinetic resolution of .beta.-hydroxy nitriles. A route to useful precursors

for .gamma.-amino alcohols

Pamies, Oscar; Backvall, Jan-E.

Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, 106 91, Swed.

Advanced Synthesis & Catalysis (2001), 343(6+7),

726-731

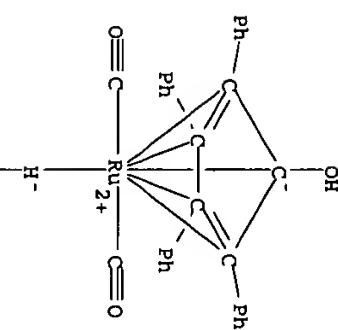
CODEN: ASCAFT; ISSN: 1615-4150

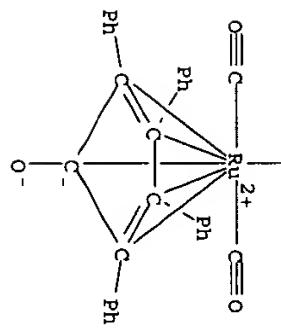
PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

PAGE 1-A



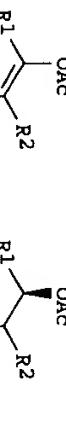


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE IN THE RE FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:416874 CAPLUS
TITLE: Stereoselective method for preparing chiral esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution
INVENTOR(S): Hyun Min Park, Jai Wook; Kim, Mahn-joo; Koh, Jeong Hwan; Jung, Family ACC. NUM. COUNT: 1

PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang University of Science and Technology
SOURCE: PCT Int. Appl., 19 pp.
DOCUMENT TYPE: Patent
LANGUAGE: English
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001040157	A1	20010607	WO 2000-KR1169	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, ID, IL, IN, IS, JP, KE, KG, KB, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1237837	A1	20020911	EP 2000-971838	20001018
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003515336	T2	20030507	JP 2001-541847	20001018
US 2001012898	A1	20010809	US 2000-726412	20001201
US 6475773	B2	20021105	KR 1999-54472	A 19991202
PRIORITY APPLN. INFO.:			WO 2000-KR1169	W 20001018
OTHER SOURCE(S):			CASREACT 135:19231; MARPAT 135:19231	GI



AB A method for prep. optically pure chiral esters I (R1, R2 and R3 = independently (un)substituted alkyl, aryl or cycloalkyl group and R1 and R2, R1 and R3, and R2 and R3 can form a cyclic ring; substituent may be halogen or cyano group) in high yield from alkenyl esters via ruthenium catalyzed redn./racemization with successive enzymic resoln. is disclosed. For example, II was synthesized in 89% yield

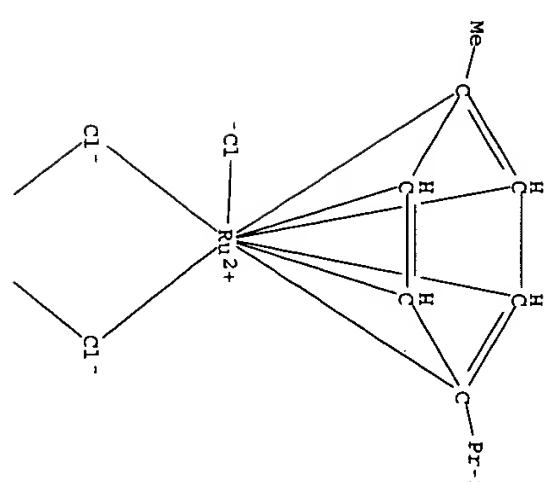
(98% enantiomeric excess) by mixing 1-phenylethynyl acetate with 2,6-dimethylheptan-4-ol, a ruthenium catalyst, and Novozym 435 followed by heating under Argon with subsequent chromatog. purifn. The chiral esters obtained can be used as synthetic intermediates for prep. various chiral compds., chiral pharmaceutical drugs (e.g. L-Carnitine) or chiral agrochems. (e.g. L-Carnitine).

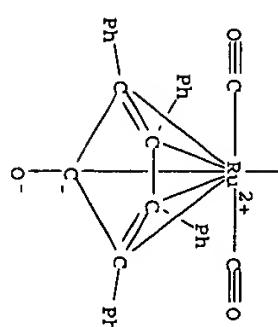
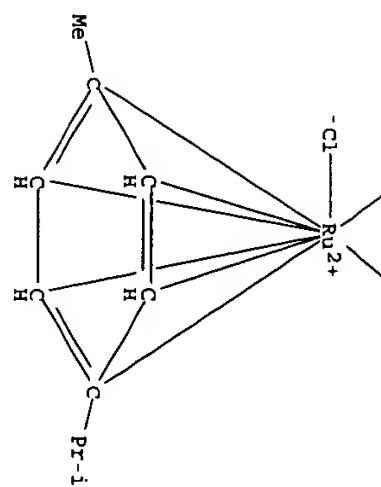
IT 9001-62-1, Novozym 52462-29-0 104439-77-2
RL: CAT (Catalyst use); USES (Uses)
(stereoselective method for prep. chiral esters from alkenyl esters via ruthenium catalyzed redn. and enzymic resoln. of racemic alc. intermediate)

RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 52462-29-0 CAPLUS
Ruthenium, di-*mu*-chlorodichlorobis((1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene)di-(9CI) (CA INDEX NAME)





REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE IN THE RE FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RN 104439-77-2 CAPIUS
 CN Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5-.eta.)-1-hydroxylato-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-.eta.)-1-hydroxy-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

AUTHOR(S):

Mi-Jung, Park, Jaiwook
 National Research Laboratory of Chirotechnology
 Department of Chemistry Division of Molecular and Life
 Sciences, Pohang University of Science and Technology,
 Pohang Kyungbuk, 790-784, S. Korea

JOURNAL: Journal of Organic Chemistry (2001), 66(13), 4736-4738
 CODEN: JOCEAH; ISSN: 0022-3263

SOURCE:

CORPORATE SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

AB The racemic title substrates were modified with bulky protecting dynamic groups and then subjected to the lipase/ruthenium-catalyzed dynamic kinetic resolin. (DKR). E.g., DKR of MeCH(OH)CH₂CO₂CH₂Ph with Pseudomonas cepacia lipase, a Ru catalyst, and 4-C₁₂CH₄OAc gave (R)-MeCH(OAc)CH₂CO₂CH₂Ph (88% yield, 86% ee).

IT 9001-62-1, lipase PSD 104439-77-2

RL: CAI (Catalyst use); USES (uses)

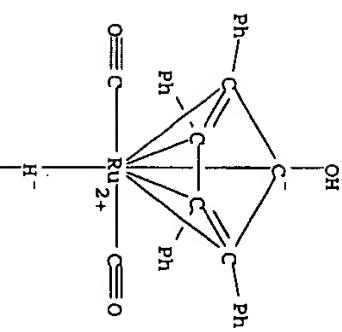
(lipase/ruthenium-catalyzed dynamic kinetic resolin of hydroxy acids, diols, and hydroxy aldehydes protected with a bulky group)

RN 9001-62-1 CAPIUS
 CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

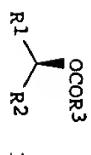
RN 104439-77-2 CAPIUS
 CN Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5-.eta.)-1-hydroxylato-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-.eta.)-1-hydroxy-
 2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

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AB Title esters [I; R₁-R₃ = (cyclo)alkyl, aryl, etc.] were prepd. from RICOR2 in the presence of a Ru complex, a lipase, a hydride donor, and an acyl donor wherein unacylated alkanol enantiomer is **racemized** providing for complete conversion.
IT 52462-29-0
RL: CAT (Catalyst use); USES (Uses)
(prepn. of chiral esters)
RN 52462-29-0 CAPLUS
CN Ruthenium, di-*mu*-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)

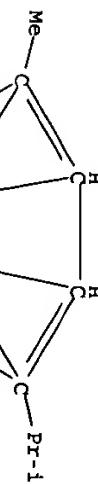


REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE IN THE RE FORMAT

LS ANSWER 16 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:300657 CAPLUS
134:310984
TITLE: Preparation of chiral esters
INVENTOR(S): Park, Jai Wook; Kim, Mahn-joo; Koh, Jeong Hwan; Jung, Hyun Min
PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang University of Science and Technology
SOURCE: PCT Int. Appl., 20 pp.
DOCUMENT TYPE: Patent
CODEN: PIXXD2
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

PAGE 1-A



AUTHOR(S): Kinetic Resolution
CORPORATE SOURCE: Huerta, Fernando F.; Baeckvall, Jan-E.
SOURCE: Department of Organic Chemistry Arrhenius Laboratory,
Stockholm University, Stockholm, SE-106 91, Swed.
CODEN: ORLEFT; **ISSN:** 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:366391

AB Combining dynamic kinetic **resoln.** with an aldol reaction provides access to .beta.-hydroxy ester derivs. with high enantiomeric purity (up to 99% ee) in a one-pot procedure. Only simple starting materials are required in this enantioselective process, and preformation of a silyl enol ether is not necessary.

IT 9001-62-1, Lipase 104439-77-2

RL: CAT (Catalyst use); **USES** (Uses)

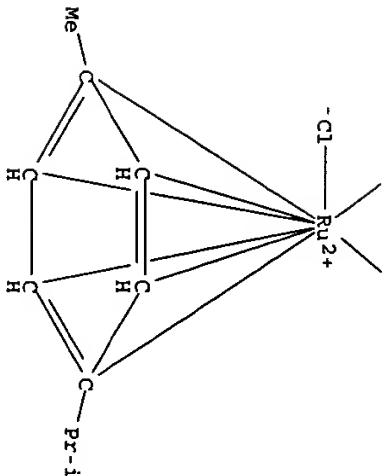
(enantioselective synthesis of .beta.-hydroxy acid derivs. via a

one-pot aldol reaction-dynamic kinetic **resoln.**)

RN 104439-77-2, CAPLUS

CN Ruthenium, tetracarbonyl-.mu.-hydro[(1,2,3,4,5-.eta.)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-.eta.)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (9CI) (CA INDEX NAME)

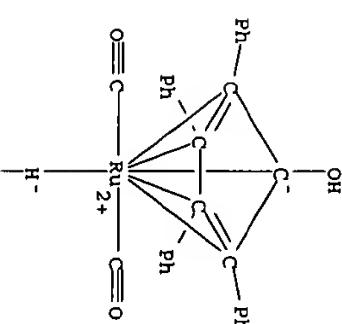
PAGE 2-A



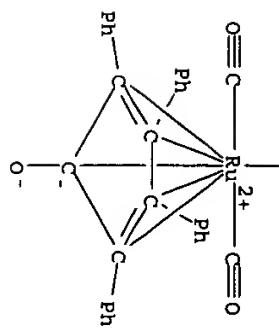
IT 9001-62-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(prep. of chiral esters)
RN 9001-62-1, CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

PAGE 1-A



L5 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:192974 CAPLUS
DOCUMENT NUMBER: 134:366391
TITLE: Enantioselective Synthesis of .beta.-Hydroxy Acid



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE IN THE RE FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:455856 CAPLUS
DOCUMENT NUMBER: 133:222192

TITLE: Dynamic Kinetic Resolution of Allylic Alcohols Mediated by Ruthenium- and Lipase-Based

Catalysts

AUTHOR(S): Lee, Donghyun; Huh, Eun A.; Kim, Mahn-Joo; Jung, Hyun Min; Koh, Jeong Hwan; Park, Jaiwook

Department of Chemistry Division of Molecular and Life Science, Pohang University of Science and Technology, Pohang Kyungbuk, 790-784, S. Korea

Organic Letters (2000), 2(15), 2377-2379

SOURCE: CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: CASREACT 133:222192
LANGUAGE: English
OTHER SOURCE(S): Journal

AB An enzyme-metal combo reaction has been developed for the dynamic kinetic resolution of allylic alcs. in which **racemic** substrates are transformed by a lipase and a ruthenium complex in the presence of an acyl donor to allylic acetates of high optical purity in over 80% yield.

IT 9001-62-1, Lipase

RL: CAT (Catalyst use); USES (Uses)

(catalyst for enantioselective acylation of **racemic** allylic alcs.; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of **racemic** allylic alcs. and Ru-catalyzed

racemization of unreacted substrate)

RN 9001-62-1 CAPIUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

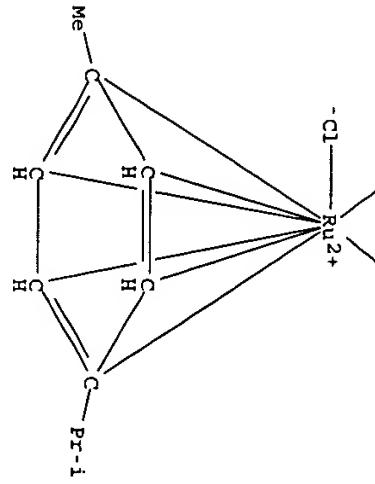
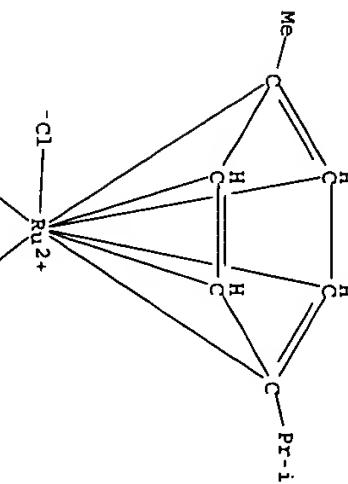
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT 52462-29-0, (p-Cymene)ruthenium(II) chloride dimer
90720-60-8, Ruthenium, .mu.-chlorodichloro-.mu.-hydrobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di-

RL: CAT (Catalyst use); USES (Uses)

(racemization catalyst for dynamic kinetic **resoln** of allylic alcs.; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of **racemic** allylic alcs. and Ru-catalyzed **racemization** of unreacted substrate)

RN 52462-29-0 CAPIUS
CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)



RN 90720-60-8 CAPIUS
CN Ruthenium, .mu.-chlorodichloro-.mu.-hydrobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)

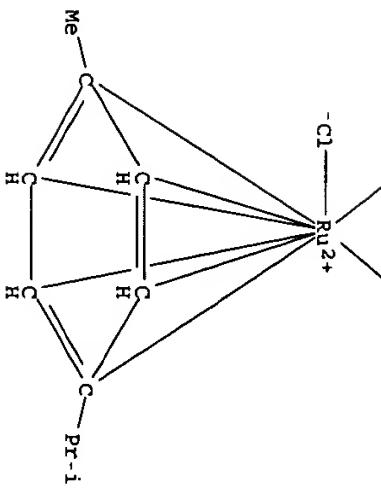
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE (S): CASREACT 132:333983
GI



IT
9001-62-1, Lipase 52462-29-0
RL: CAT (Catalyst use); USES (Uses)
(nonracemic prepn. of .alpha.-hydroxy esters by dynamic resoln
. in the presence of *Pseudomonas cepacia* lipase and a diruthenium catalyst)
9001-62-1 CAPIUS

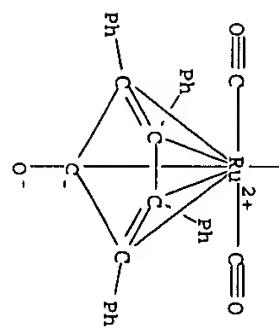
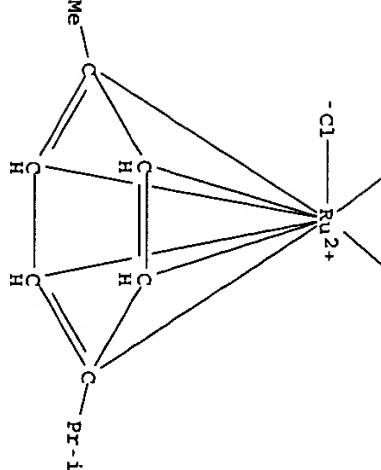
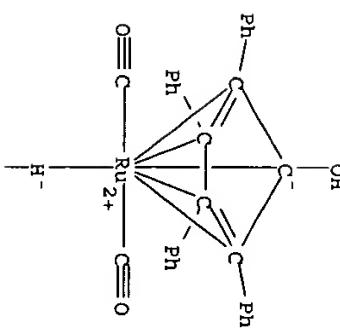
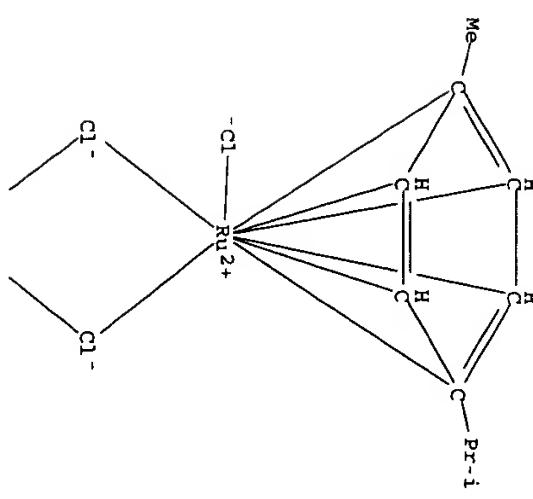
RN
CN
Lipase, triacylglycerol (9CI) (CA INDEX NAME)
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN
CN
52462-29-0 CAPIUS
Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 19 OF 23 CAPIUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:196518 CAPIUS
DOCUMENT NUMBER: 132:333983
TITLE: Dynamic Kinetic Resolution of .alpha.-Hydroxy Acid Esters
AUTHOR (S): Huerta, Fernando F.; Laxmi, Y. R. Santosh; Baeckvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry Arhenius Laboratory, Stockholm University, Stockholm, SE-106 91, Swed.
Organic Letters (2000), 2(8), 1037-1040
SOURCE: CODEN: ORLEFT; ISSN: 1523-7060

104439-77-2P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP(Preparation); RACT (Reactant or reagent); USES (Uses)
(nonracemic prepn. of .alpha.-hydroxy esters by dynamic resolin

. in the presence of Pseudomonas cepacia lipase and a diruthenium

catalyst)

RN 104439-77-2 CAPLUS

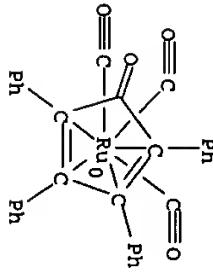
CN RUTHENIUM, TETRACARBONYL-.mu.-HYDRO[1,2,3,4,5-.eta.]-1-HYDROXYLATO-

2,3,4,5-TETRAPHENYL-2,4-CYCLOPENTADIEN-1-YL][(1,2,3,4,5-.eta.)-1-HYDROXY-
2,3,4,5-TETRAPHENYL-2,4-CYCLOPENTADIEN-1-YL]DI- (9CI) (CA INDEX NAME)

IT 12321-08-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation);
USES (Uses)
(nonracemic prepn. of .alpha.-hydroxy esters by dynamic resolin
. in the presence of Pseudomonas cepacia lipase and a diruthenium
catalyst)

RN 12321-08-3 CAPLUS

CN RUTHENIUM, TRICARBONYL[(2,3,4,5-.eta.)-2,3,4,5-TETRAPHENYL-2,4-
CYCLOPENTADIEN-1-ONE]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

17

THERE ARE 17 CITED REFERENCES AVAILABLE IN THE RE FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:379055
DOCUMENT NUMBER: 131:129567TITLE: Dynamic Kinetic Resolution of Secondary
Diols via Coupled Ruthenium and Enzyme Catalysis

AUTHOR(S): Persson, B. Anders; Huerta, Fernando F.; Baeckvall,

Jan-E.

Department of Organic Chemistry, Uppsala University,

Uppsala, SE-751 21, Swed.

Journal of Organic Chemistry (1999), 64(14), 5237-5240

CORPORATE SOURCE: CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:129567

AB Enzymic acylation of secondary sym. diols (as meso/dL mixts.) in combination with ruthenium-catalyzed isomerization of the diol led to efficient dynamic kinetic resoln. In this way, a meso/dL mixt. of the diol was transformed to enantiomerically pure (R,R)-diacetate, making efficient use of all the diol material. For some of the flexible substrates, substantial amounts of meso-diacetates were formed as side products. The results indicate that the major part of the meso product is formed via an intramol. acyl-transfer pathway.

IT 9001-62-1, Novozym 435 104439-77-2

RL: CAT (Catalyst use); USES (Uses)

(dynamic kinetic resoln. of secondary diols via coupled

ruthenium and enzyme catalysis)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (GCI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 104439-77-2 CAPLUS

CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.]-1-hydroxylato-

2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][1,2,3,4,5-.eta.]-1-hydroxy-

2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di- (GCI) (CA INDEX NAME)

REFERENCE COUNT:

29

THERE ARE 29 CITED REFERENCES AVAILABLE IN THE RE FORMAT RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:332954 CAPLUS
DOCUMENT NUMBER: 129:95085TITLE: Asymmetric Diels-Alder reaction via enzymic kinetic
resolution using ethoxyvinyl methyl fumarate

AUTHOR(S): Kita, Yasuyuki; Imanishi, Masashi; Akai, Shuji;

CORPORATE SOURCE: Matsugi, Masato

SOURCE: Graduate School of Pharmaceutical Sciences, Osaka

University, Osaka, 565, Japan

Chemical Communications (Cambridge) (1998), (11),

1183-1184

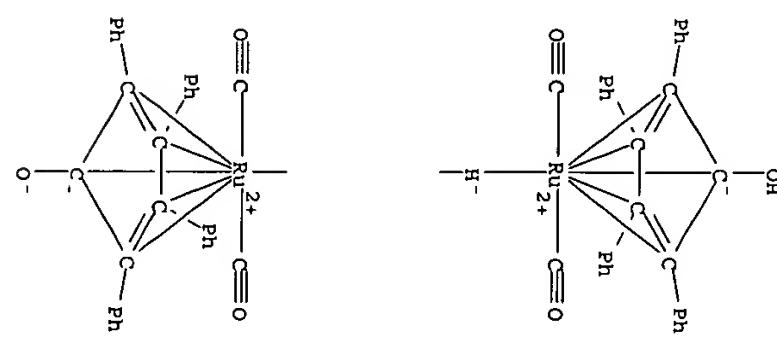
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A domino-type asym. [4+2] cycloaddn. reaction following TOYOBO LIP



enzymic kinetic **resoln.** using ethoxyvinyl Me fumarate is described.

IT 9001-62-1, Lipase 52462-29-0

RL: CAT (Catalyst use); USES (Uses)
(asym. Diels-Alder reaction via enzymic kinetic **resoln.** using

ethoxyvinyl Me fumarate)

RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 52462-29-0 CAPLUS

CN Ruthenium, di-.mu.-chlorodichlorobis[(1,2,3,4,5,6-.eta.)-1-methyl-4-(1-methylethyl)benzene]di- (9CI) (CA INDEX NAME)

PAGE 1-A

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:16459 CAPLUS
DOCUMENT NUMBER: 128:23109

Synthesis of 4-Sulfur-Substituted (2S,3R)-3-Phenylserines by Enzymic Resolution. Enantiopure Precursors for Thiamphenicol and Florfenicol

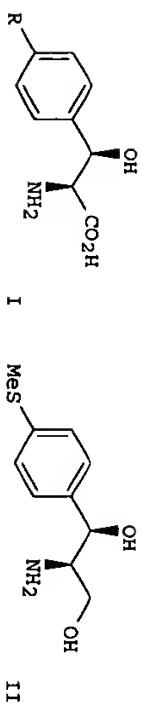
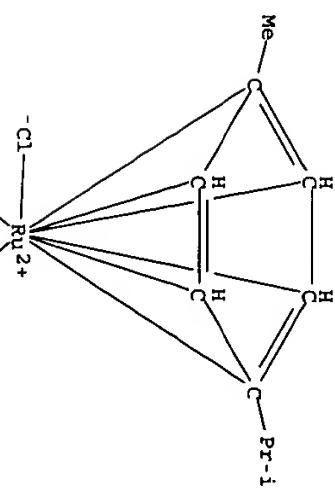
Kaptein, Bernard; van Dooren, Thei J. G. M.; Boesten, L.; Broxterman, Quirinus B.; Kamphuis, Johan Wilhelmus H. J.; Sonke, Theo; Duchateau, Alexander L. Chemicals, DSM Research, Geleen, 6160 MD, Neth.

Organic Process Research & Development (1998), 2(1), 10-17

CODEN: OPRDFK; ISSN: 1083-6160
American Chemical Society
Journal

LANGUAGE: English

CASREACT 128:23109



AB Enantiomerically pure 4-methylthio- and 4-methylsulfonyl-substituted

(2S,3R)-3-phenylserines I (R = MeS, MesO2) are prep'd. by enzymic **resoln.** of the corresponding **racemic** threo amides using the amidase from *Ochrobactrum anthropi* NCIMB 40321. The unwanted (2R,3S)-amide enantiomers are sep'd. from the enantiopure amino acids and easily **racemized** after Schiff base formation with the corresponding 4-(methylthio)- and 4-(methylsulfonyl)benzaldehyde. The **racemization** can be combined with the prepn. of the **racemic** amides by aldol reaction under crystn. conditions to yield only the threo isomers. Enantiopure phenylserines I (R = MeS, MesO2) are thus obtained in 78% and 62% overall yields starting from the corresponding substituted aldehydes. I (R = MeS) is reduced to diol II with NABH4/H2SO4 and can be used for the synthesis of thiamphenicol and florfenicol.

IT 9001-62-1, Lipase 109361-17-3

RL: CAT (Catalyst use); USES (Uses)
(asym. synthesis of sulfur-substituted phenylserines by enzymic **resoln.** of **racemic** amides and **racemization** of unwanted stereoisomers)

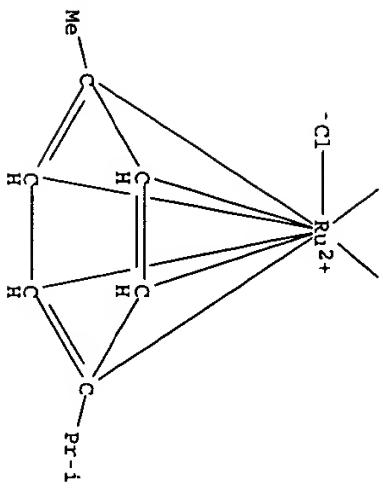
RN 9001-62-1 CAPLUS

CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 109361-17-3 CAPLUS

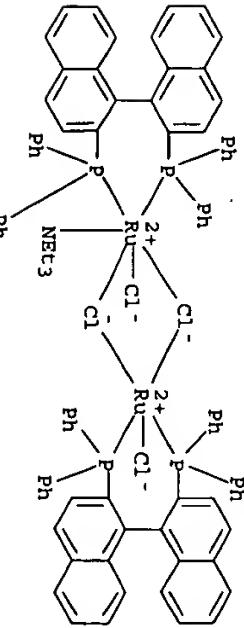
CN Ruthenium, bis[(IR)-[1,1'-binaphthalene]-2,2'-diylbis(diphenylphosphine-kappa-P)]di-.mu.-chlorodichloro(N,N-diethylethananamine)di- (9CI) (CA INDEX NAME)



PAGE 2-A

CN Ruthenium, tetracarbonyl-.mu.-hydro[1,2,3,4,5-.eta.]-1-hydroxylato-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl] [(1,2,3,4,5-.eta.)-1-hydroxy-
2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl] di- (9CI) (CA INDEX NAME)

PAGE 1-A



REFERENCE COUNT:

34

THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:407237 CAPLUS
DOCUMENT NUMBER: 127:135610

TITLE: Enzymic resolution of alcohols coupled with ruthenium-catalyzed racemization of the substrate alcohol

AUTHOR(S): Larsson, Anna L. E.; Persson, B. Anders; Backvall, Jan-E.

CORPORATE SOURCE: Department Organic Chemistry, Uppsala University, Uppsala, S-75121, Swed.

SOURCE: Angewandte Chemie, International Edition in English (1997), 36(11), 1211-1212

CODEN: ACIEAY; ISSN: 0570-0833

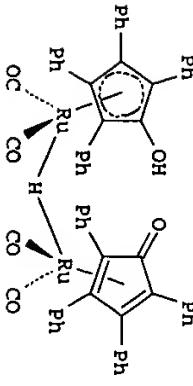
PUBLISHER: Wiley-VCH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:135610

GI



AB The ruthenium-catalyzed racemization of (+)-(R)-.alpha.-methylbenzenemethanol was coupled with an enzyme-catalyzed

transesterification to give the resolved alc. deriv. Thus, the combination of catalyst I, 4-chlorophenyl acetate and Novozym 435 in the reaction of (+)-(R)-.alpha.-methylbenzenemethanol gave (R)-.alpha.-methylbenzenemethanol acetate in high yield and high enantiomeric purity.

IT 9001-62-1, Novozym 435 104439-77-2

RL: CAT (Catalyst use); USES (Uses (ruthenium-catalyzed racemization and sequential enzymic resoln. of alcs.))

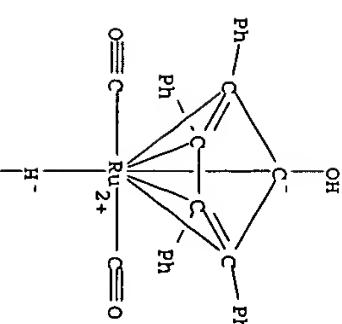
RN 9001-62-1 CAPLUS
CN Lipase, triacylglycerol (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 104439-77-2 CAPLUS

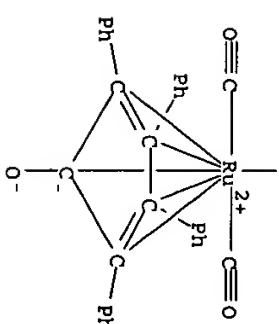
REFERENCE COUNT:

41

THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



PAGE 2-A



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